

=> fil casre; d stat que l46

FILE 'CASREACT' ENTERED AT 12:44:19 ON 27 MAY 2005

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FILE CONTENT:1840 - 22 May 2005 VOL 142 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 9.2 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L43

STR

RRT = reagent or reactant
RRT
Cb—P
1 2

PRO = product
PRO PRO
O=C=N O=C=N
4 5 6 12 13 14

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 2 - *Phosphorus at node 2 is connected to exactly 3 non-hydrogen atoms*
CONNECT IS E2 RC AT 5
CONNECT IS M2 RC AT 6
CONNECT IS E2 RC AT 13
CONNECT IS M2 RC AT 14
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 1 - *Carbocycle at node 1 is saturated*
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L46 0 SEA FILE=CASREACT SSS FUL L43 (0 REACTIONS)

100.0% DONE 1333 VERIFIED

0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

```
=> fil casrea; d stat que l49
FILE 'CASREACT' ENTERED AT 12:44:33 ON 27 MAY 2005
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```

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FILE CONTENT:1840 - 22 May 2005 VOL 142 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 9.2 million reactions      *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
L47          STR
              PRO          PRO
RRT          O=C=N        O=C=N
              4   5   6    12 13 14
```

Cb—P

1 2

any carbocycle (saturated or unsaturated)

NODE ATTRIBUTES:

```
CONNECT IS E3 RC AT 2
CONNECT IS E2 RC AT 5
CONNECT IS M2 RC AT 6
CONNECT IS E2 RC AT 13
CONNECT IS M2 RC AT 14
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

```
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8
```

STEREO ATTRIBUTES: NONE

L49 7 SEA FILE=CASREACT SSS FUL L47 (34 REACTIONS)

```
100.0% DONE 1333 VERIFIED 34 HIT RXNS 7 DOCS
SEARCH TIME: 00.00.01
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=> d ibib abs hit 1-7

COMMAND INTERRUPTED
REENTER FILE 'CASREACT'
AND TRY AGAIN, OR ENTER '?' FOR MORE INFORMATION.

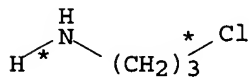
=> => d ibib abs hit 1-7

L49 ANSWER 1 OF 7 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:88898 CASREACT
TITLE: Helically chiral polymers: a class of ligands for asymmetric catalysis
AUTHOR(S): Reggelin, Michael; Doerr, Sebastian; Klussmann, Martin; Schultz, Melanie; Holbach, Michael
CORPORATE SOURCE: Institut fuer Organische Chemie, Technische Universitaet Darmstadt, Darmstadt, D-64287, Germany
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(15), 5461-5466
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Helically chiral polymers from achiral monomers containing N and P atoms have been shown to be ligands for transition metals such as Pd and Rh. The Rh complex of the phosphane-containing copolymer of H3BPPH2(CH2)3NCO and Me2CH(C.tplbond.C)3CHMeCH2NCO was an active albeit hardly enantioselective catalyst in the asym. hydrogenation of N-acetyldehydrophenylalanine (15% enantiomeric excess). The most active catalyst obtained until now was the Pd-complexed polymer of 4-H3BPPH2C6H4CPh2O2CCMe:CH2, which catalyzes the allylic substitution reaction of 1,3-diphenylprop-2-enyl acetate with di-Me malonate even at -20°C in quant. yield, although again the enantioselectivity was unsatisfactory. The most successful application of a helically chiral polymer in asym. catalysis with respect to both reactivity and enantioselectivity is the copolymer of phenylbis(2-pyridinyl)methyl methacrylate with trityl methacrylate. Its palladium complex catalyzes the above-mentioned reaction at 0°C with quant. yield and 60% enantiomeric excess.

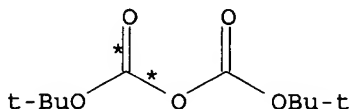
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(27) OF 30 COMPOSED OF RX(11), RX(12), RX(13), RX(10)
RX(27) AL + AM + AN + AU + AH + AI ==> AD

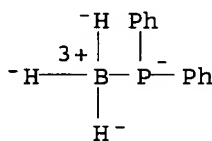


● HCl

AL

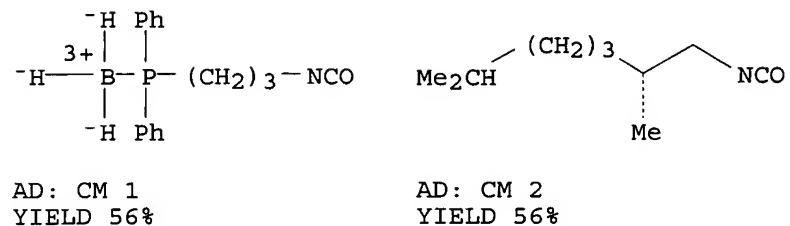
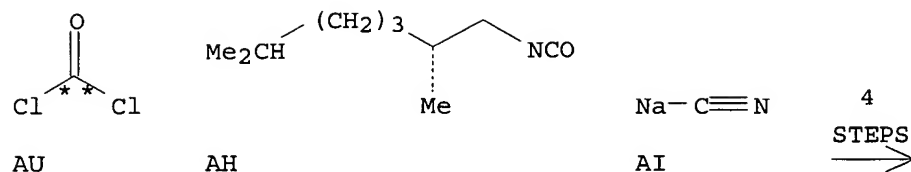


AM



● Li+

AN



RX(11) RCT AL 6276-54-6, AM 24424-99-5

STAGE(1)

RGT AP 144-55-8 NaHCO₃

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RCT AN 145130-18-3

SOL 109-99-9 THF

PRO AO 713542-60-0

RX(12) RCT AO 713542-60-0

RGT AT 75-36-5 AcCl

PRO AS 713542-61-1

SOL 67-56-1 MeOH

RX(13) RCT AS 713542-61-1

STAGE(1)

RGT AP 144-55-8 NaHCO₃

SOL 7732-18-5 Water, 67-66-3 CHCl₃

STAGE(2)

RCT AU 75-44-5

SOL 108-88-3 PhMe

PRO AG 713542-58-6

RX(10) RCT AG 713542-58-6, AH 122093-49-6

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT AJ 143-66-8 Na Ph₄B

SOL 109-99-9 THF

STAGE(3)

RCT AI 143-33-9

SOL 68-12-2 DMF

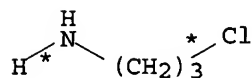
STAGE(4)

RGT AF 7647-01-0 HCl

SOL 67-56-1 MeOH

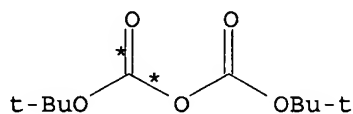
PRO AD 713542-59-7

RX(30) OF 30 COMPOSED OF RX(11), RX(12), RX(13), RX(10), RX(9)
 RX(30) AL + AM + AN + AU + AH + AI ==> AE

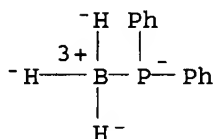


● HCl

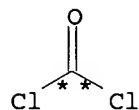
AL



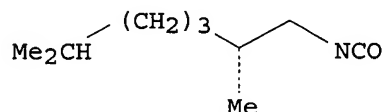
AM

● Li⁺

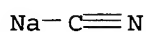
AN



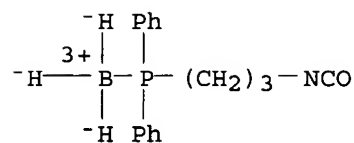
AU



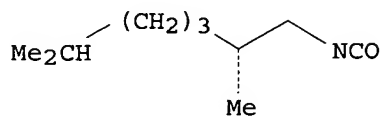
AH



AI

5
STEPS
→

AE: CM 1
 YIELD 92%



AE: CM 2
 YIELD 92%

RX(11) RCT AL 6276-54-6, AM 24424-99-5

STAGE(1)

RGT AP 144-55-8 NaHCO₃

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RCT AN 145130-18-3

SOL 109-99-9 THF

PRO AO 713542-60-0

RX(12) RCT AO 713542-60-0
 RGT AT 75-36-5 AcCl

PRO AS 713542-61-1
SOL 67-56-1 MeOH

RX(13) RCT AS 713542-61-1

STAGE(1)
RGT AP 144-55-8 NaHCO₃
SOL 7732-18-5 Water, 67-66-3 CHCl₃

STAGE(2)
RCT AU 75-44-5
SOL 108-88-3 PhMe
PRO AG 713542-58-6

RX(10) RCT AG 713542-58-6, AH 122093-49-6

STAGE(1)
SOL 109-99-9 THF

STAGE(2)
RGT AJ 143-66-8 Na Ph₄B
SOL 109-99-9 THF

STAGE(3)
RCT AI 143-33-9
SOL 68-12-2 DMF

STAGE(4)
RGT AF 7647-01-0 HCl
SOL 67-56-1 MeOH
PRO AD 713542-59-7

RX(9) RCT AD 713542-59-7
RGT AB 280-57-9 Triethylenediamine, AF 7647-01-0 HCl
PRO AE 713542-59-7D
SOL 67-56-1 MeOH, 109-99-9 THF, 108-88-3 PhMe

L49 ANSWER 2 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:36622 CASREACT

TITLE: Ruthenium(II) and Ruthenium(IV) Complexes Containing
 κ^1 -P-, κ^2 -P,O-, and κ^3 -P,N,O-
Iminophosphorane-Phosphine Ligands

AUTHOR(S): Ph₂PCH₂P{ :NP(:O)(OR)₂ }Ph₂ (R = Et, Ph): Synthesis,
Reactivity, Theoretical Studies, and Catalytic
Activity in Transfer Hydrogenation of Cyclohexanone
Cadierno, Victorio; Crochet, Pascale; Diez, Josefina;
Garcia-Alvarez, Joaquin; Garcia-Garrido, Sergio E.;
Gimeno, Jose; Garcia-Granda, Santiago; Rodriguez,
Miguel A.

CORPORATE SOURCE: Departamento de Quimica Organica e Inorganica,
Instituto Universitario de Quimica Organometalica
Enrique Moles (Unidad Asociada al CSIC), Facultad de
Quimica, Universidad de Oviedo, Oviedo, E-33071, Spain

SOURCE: Inorganic Chemistry (2003), 42(10), 3293-3307
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

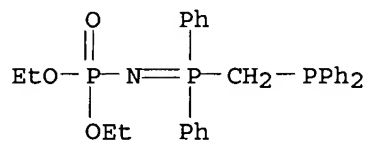
LANGUAGE: English

AB [{Ru(η^6 -p-cymene)(μ -Cl)Cl}₂] and [{Ru(η^3 : η^3 -C₁₀H₁₆)(μ -

Cl)Cl}2] react with Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂ (R = Et (1a), Ph (1b)) affording complexes [Ru(η⁶-p-cymene)Cl₂(κ¹-P-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] (R = Et (2a), Ph (2b)) and [Ru(η³:η³-C₁₀H₁₆)Cl₂(κ¹-P-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] (R = Et (6a), Ph (6b)). While treatment of 2a with 1 equivalent of AgSbF₆ yields a mixture of [Ru(η⁶-p-cymene)Cl(κ²-P,O-Ph₂PCH₂P{:NP(:O)(OEt)₂}Ph₂)] [SbF₆] (3a) and [Ru(η⁶-p-cymene)Cl(κ²-P,N-Ph₂PCH₂P{:NP(:O)(OEt)₂}Ph₂)] [SbF₆] (4a), [Ru(η⁶-p-cymene)Cl(κ²-P,O-Ph₂PCH₂P{:NP(:O)(OPh)₂}Ph₂)] [SbF₆] (3b) and [Ru(η³:η³-C₁₀H₁₆)Cl(κ²-P,O-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] [SbF₆] (R = Et (7a), Ph (7b)) are selectively formed from 2b and 6a,b. Complexes [Ru(η⁶-p-cymene)(κ³-P,N,O-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] [SbF₆]₂ (R = Et (5a), Ph (5b)) and [Ru(η³:η³-C₁₀H₁₆)(κ³-P,N,O-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] [SbF₆]₂ (R = Et (8a), Ph (8b)) have been prepared using 2 equivalent of AgSbF₆. The reactivity of 3-5a,b has been explored allowing the synthesis of [Ru(η⁶-p-cymene)X₂(κ¹-P-Ph₂PCH₂P{:NP(:O)(OR)₂}Ph₂)] (R = Et, Ph; X = Br, I, N₃, NCO (9-12a,b)). The catalytic activity of 2-8a,b in transfer hydrogenation of cyclohexanone, as well as theor. calcns. on the models [Ru(η⁶-C₆H₆)Cl(κ²-P,N-H₂PCH₂P{:NP(:O)(OH)₂}H₂)]⁺ and [Ru(η⁶-C₆H₆)Cl(κ²-P,O-H₂PCH₂P{:NP(:O)(OH)₂}H₂)]⁺, has been also studied.

REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

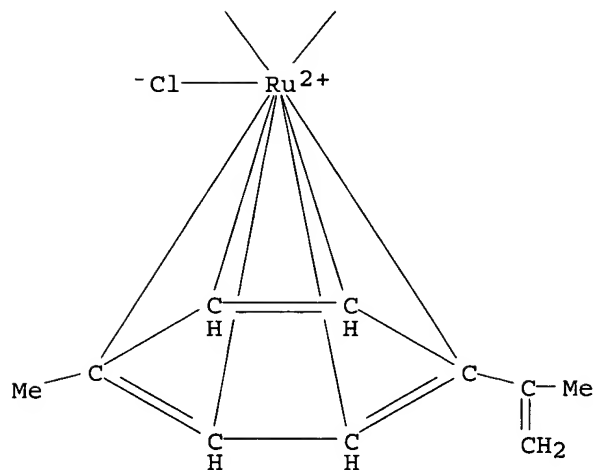
RX(37) OF 151 COMPOSED OF RX(4), RX(12)
RX(37) 2 C + 2 E + 4 W ==> 2 X



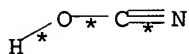
2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E



● Na

2

STEPS

4 W

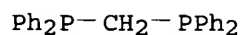
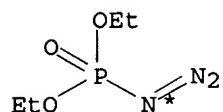
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(59) OF 151 COMPOSED OF RX(1), RX(4), RX(12)
 RX(59) 2 A + 2 B + 2 E + 4 W ==> 2 X

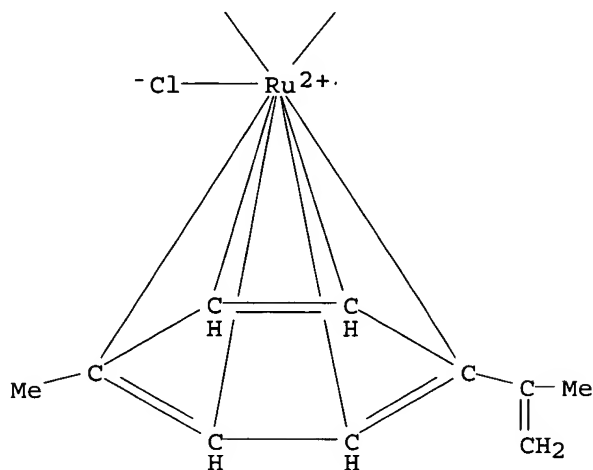


2 A

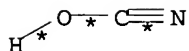
2 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E



● Na

3

STEPS
→

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

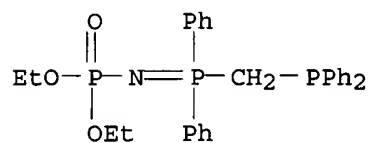
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1)	RCT	A 1516-68-3, B 2071-20-7
	PRO	C 540518-26-1
	SOL	109-99-9 THF
RX(4)	RCT	C 540518-26-1, E 135585-10-3
	RGT	J 26042-64-8 AgSbF6
	PRO	H 540518-31-8, I 540518-34-1
	SOL	75-09-2 CH2Cl2

NTE in dark, 82% overall

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
PRO X 540518-52-3
SOL 67-56-1 MeOH

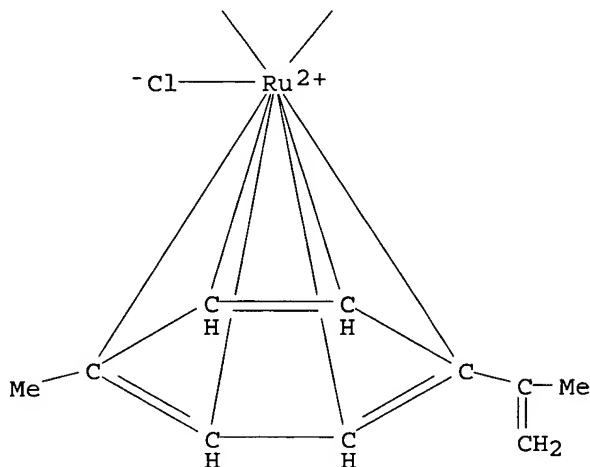
RX(65) OF 151 COMPOSED OF RX(2), RX(3), RX(12)
RX(65) 2 C + 2 E + 4 W ==> 2 X



2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

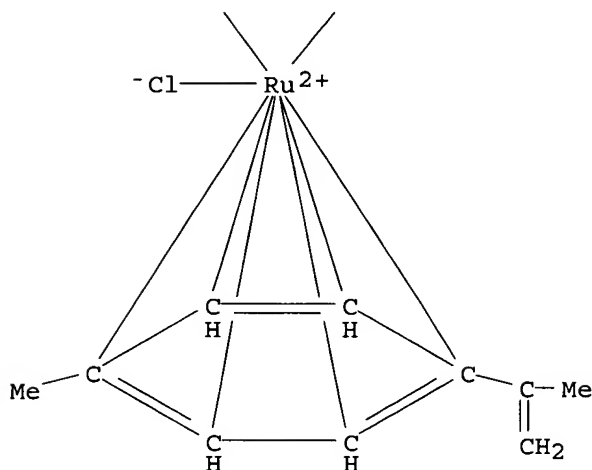
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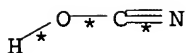
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



E



● Na

3

STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

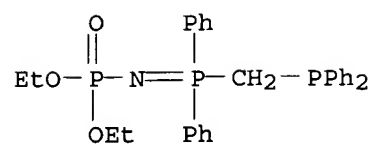
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 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(69) OF 151 COMPOSED OF RX(2), RX(5), RX(12)

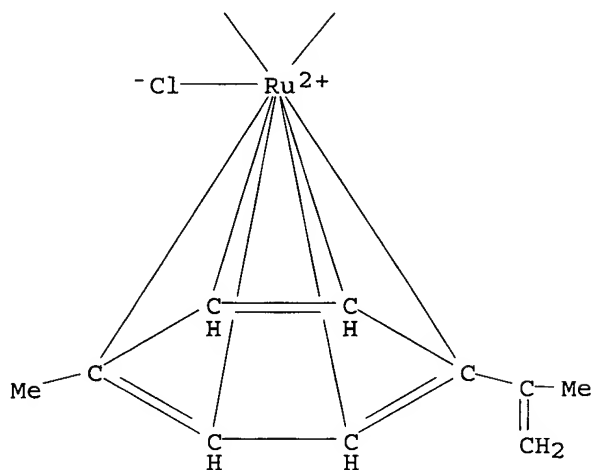
RX(69) 2 C + 2 E + H + 4 W ==> 2 X



2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

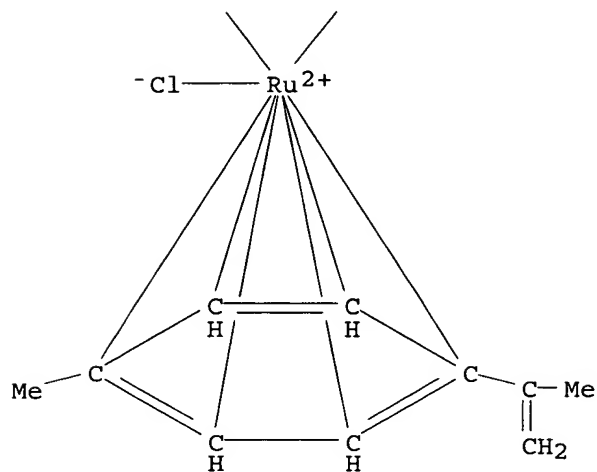
PAGE 2-A



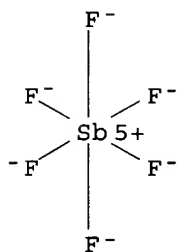
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



E

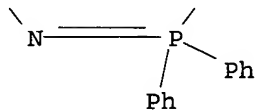


H: CM 1

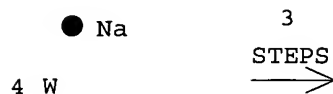
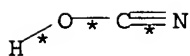
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



H: CM 2



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

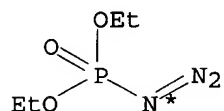
RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(73) OF 151 COMPOSED OF RX(1), RX(2), RX(3), RX(12)

RX(73) 2 A + 2 B + 2 E + 4 W ==> 2 X

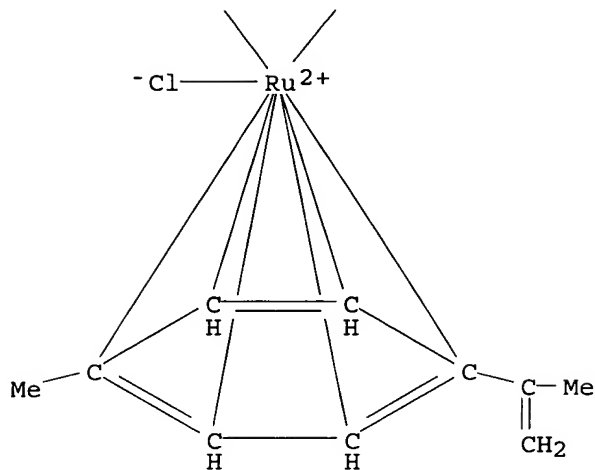


2 A

2 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

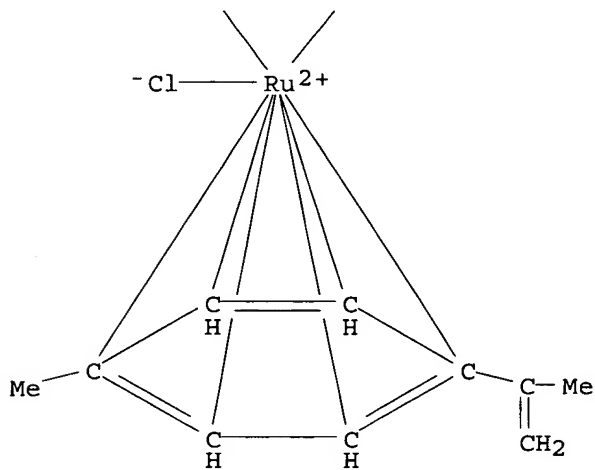
PAGE 2-A



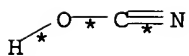
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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4

STEPS
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4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 1516-68-3, B **2071-20-7**
PRO C 540518-26-1
SOL 109-99-9 THF

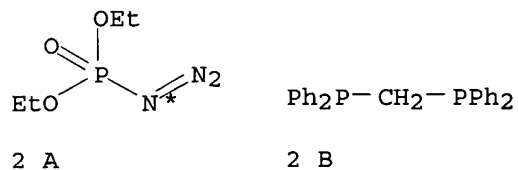
RX(2) RCT C 540518-26-1, E 135585-10-3
PRO F 540518-28-3
SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
RGT J 26042-64-8 AgSbF₆
PRO H 540518-31-8, I 540518-34-1
SOL 75-09-2 CH₂Cl₂
NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
PRO X **540518-52-3**
SOL 67-56-1 MeOH

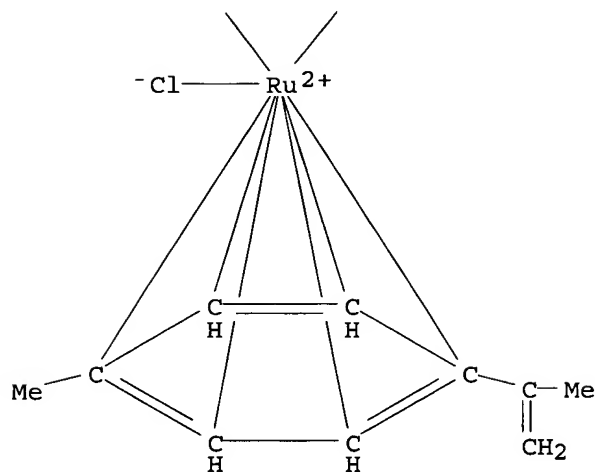
RX(77) OF 151 COMPOSED OF RX(1), RX(2), RX(5), RX(12)

RX(77) 2 A + 2 B + 2 E + H + 4 W ==> 2 X



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

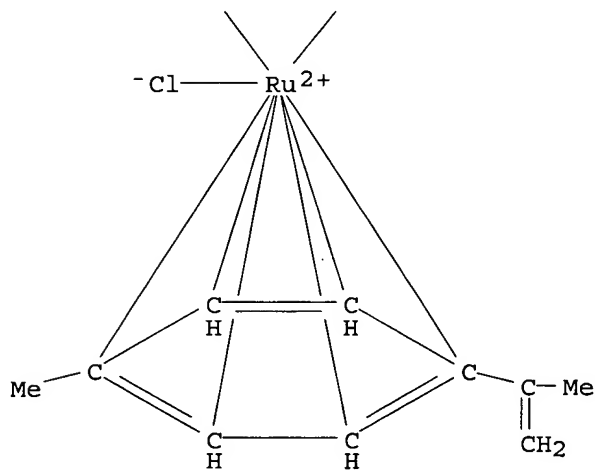
PAGE 2-A



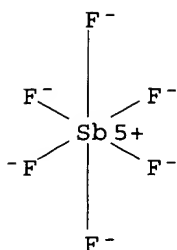
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

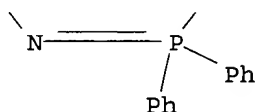


H: CM 1

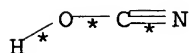
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



H: CM 2



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4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1)	RCT	A 1516-68-3, B 2071-20-7
	PRO	C 540518-26-1
	SOL	109-99-9 THF
RX(2)	RCT	C 540518-26-1, E 135585-10-3
	PRO	F 540518-28-3
	SOL	75-09-2 CH2Cl2
RX(5)	RCT	F 540518-28-3
	RGT	J 26042-64-8 AgSbF6
	PRO	K 540518-37-4, I 540518-34-1
	SOL	75-09-2 CH2Cl2
	NTE	in dark
RX(12)	RCT	H 540518-31-8, I 540518-34-1, W 917-61-3

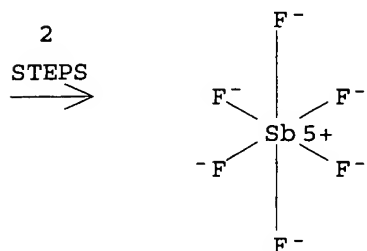
PRO X 540518-52-3
SOL 67-56-1 MeOH

RX(85) OF 151 COMPOSED OF REACTION SEQUENCE RX(5), RX(12)
AND REACTION SEQUENCE RX(4), RX(12)

...2 F ==> I...

...2 C + 2 E + 4 W ==> 2 X

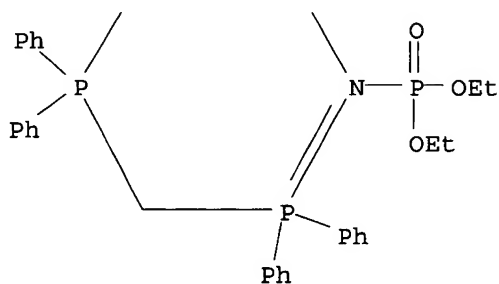
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



I: CM 1

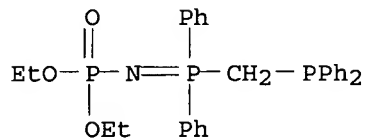
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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I: CM 2

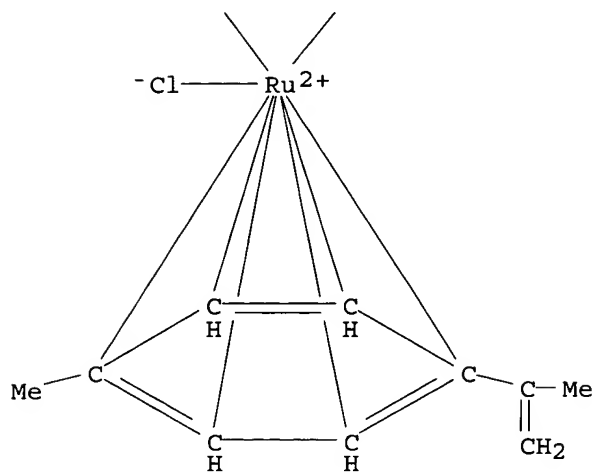
START NEXT REACTION SEQUENCE



2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

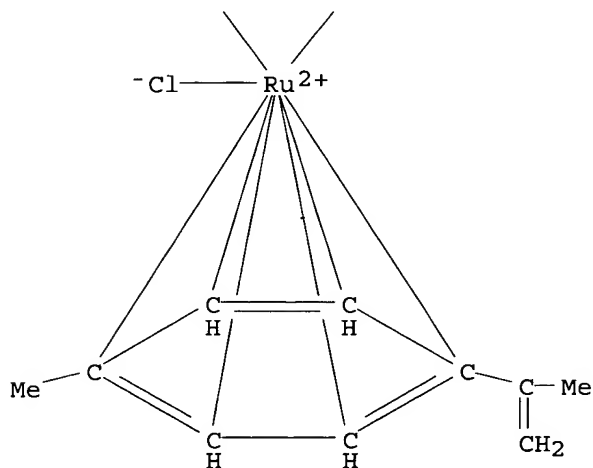
PAGE 2-A



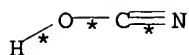
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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STEPS

4 W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

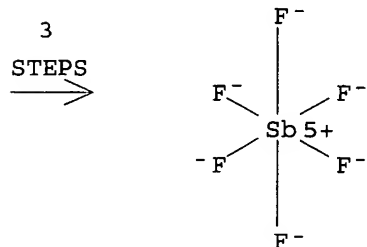
RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(89) OF 151 COMPOSED OF REACTION SEQUENCE RX(5), RX(12)
 AND REACTION SEQUENCE RX(1), RX(4), RX(12)

...2 F ==> I...

...A + B + 2 E + 4 W ==> 2 X

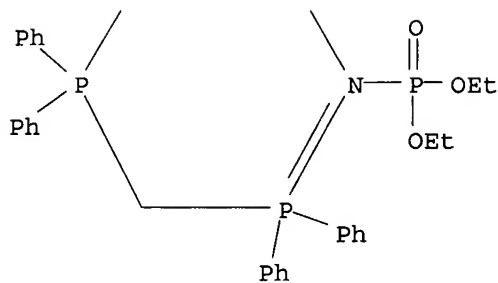
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



I: CM 1

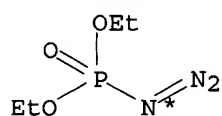
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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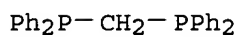


I: CM 2

START NEXT REACTION SEQUENCE



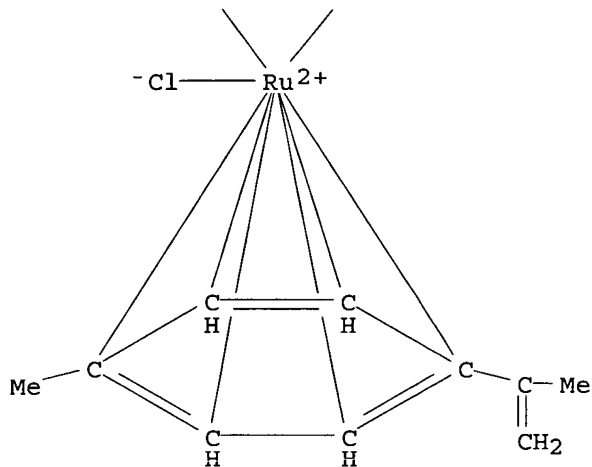
A



B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

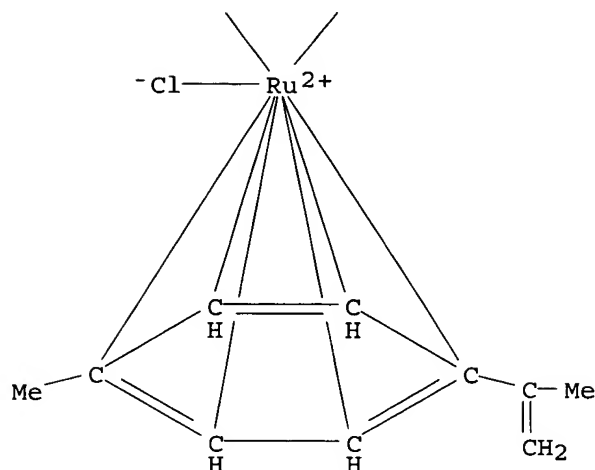
PAGE 2-A



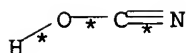
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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3

STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

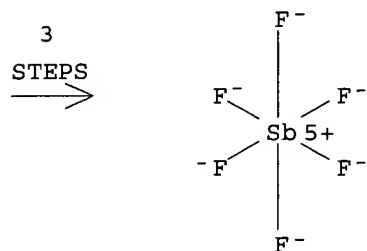
RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(93) OF 151 COMPOSED OF REACTION SEQUENCE RX(5), RX(12)
AND REACTION SEQUENCE RX(2), RX(3), RX(12)

...2 F ==> I...

... C + E + 4 W ==> 2 X

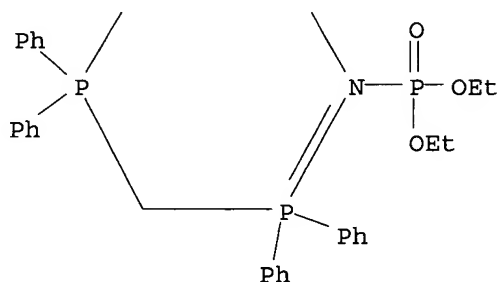
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



I: CM 1

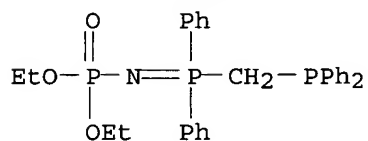
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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I: CM 2

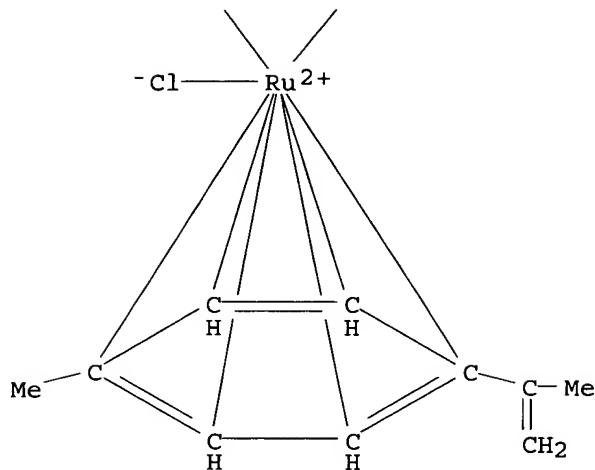
START NEXT REACTION SEQUENCE



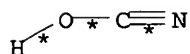
C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

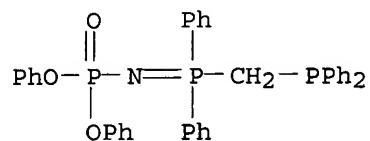
RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(100) OF 151 COMPOSED OF RX(14), RX(15), RX(23)

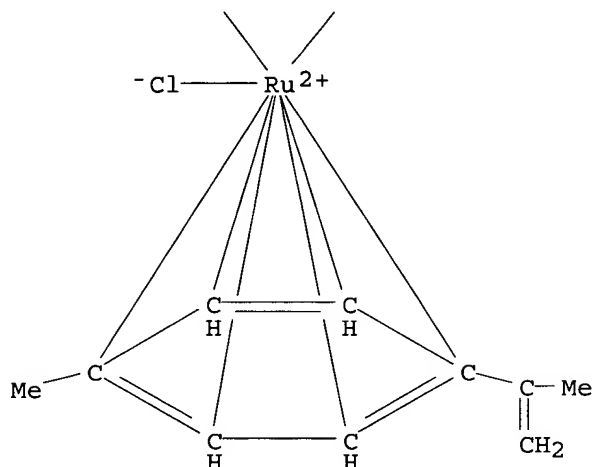
RX(100) Z + E + 2 W ==> AJ



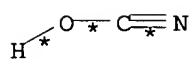
Z

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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2 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

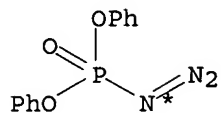
RX(14) RCT Z 540518-54-5, E 135585-10-3
PRO AA 540518-56-7
SOL 75-09-2 CH2Cl2

RX(15) RCT AA 540518-56-7
RGT J 26042-64-8 AgSbF6

PRO AB 540518-59-0
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(23) RCT AB 540518-59-0, W 917-61-3
 PRO AJ 540518-77-2
 SOL 67-56-1 MeOH

RX(105) OF 151 COMPOSED OF RX(13), RX(14), RX(15), RX(23)
 RX(105) Y + B + E + 2 W ==> AJ

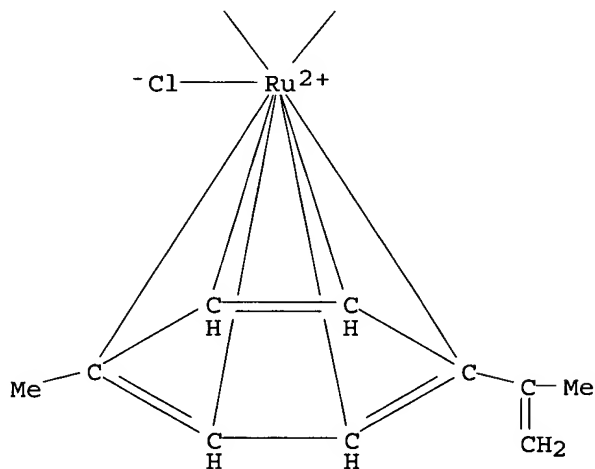


Y

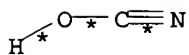
B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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2 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(13) RCT Y 26386-88-9, B 2071-20-7
 PRO Z 540518-54-5
 SOL 109-99-9 THF

RX(14) RCT Z 540518-54-5, E 135585-10-3
 PRO AA 540518-56-7
 SOL 75-09-2 CH₂Cl₂

RX(15) RCT AA 540518-56-7
 RGT J 26042-64-8 AgSbF₆
 PRO AB 540518-59-0
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

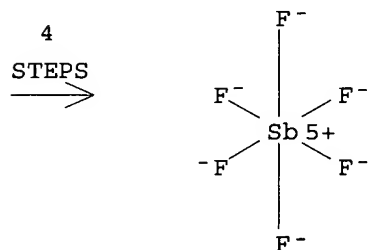
RX(23) RCT AB 540518-59-0, W 917-61-3
 PRO AJ 540518-77-2
 SOL 67-56-1 MeOH

RX(111) OF 151 COMPOSED OF REACTION SEQUENCE RX(5), RX(12)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(12)

...2 F ==> I...

...A + B + E + 4 W ==> 2 X

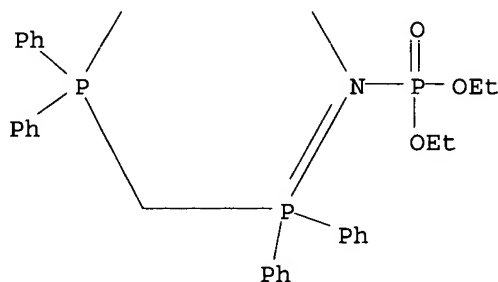
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



I: CM 1

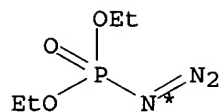
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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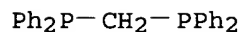


I: CM 2

START NEXT REACTION SEQUENCE



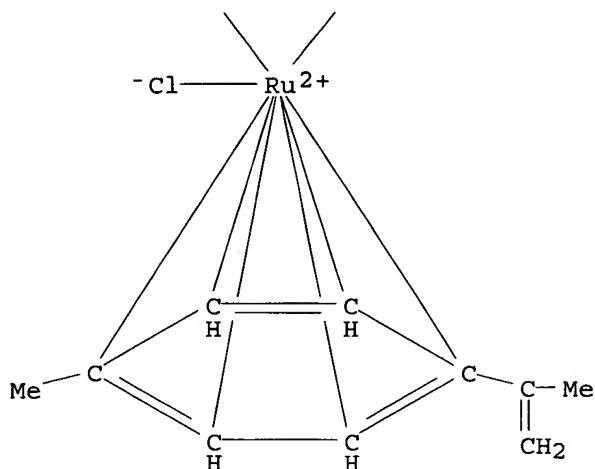
A



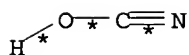
B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
PRO F 540518-28-3
SOL 75-09-2 CH₂Cl₂

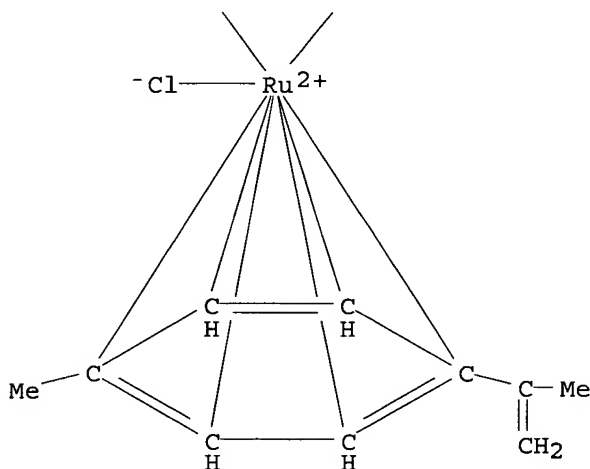
RX(3) RCT F 540518-28-3
RGT J 26042-64-8 AgSbF₆
PRO H 540518-31-8, I 540518-34-1
SOL 75-09-2 CH₂Cl₂
NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
PRO X 540518-52-3
SOL 67-56-1 MeOH

RX(115) OF 151 COMPOSED OF REACTION SEQUENCE RX(4), RX(12)
AND REACTION SEQUENCE RX(2), RX(5), RX(12)
...3 C + 3 E ==> H + I...
... C + E + H + 4 W ==> 2 X

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

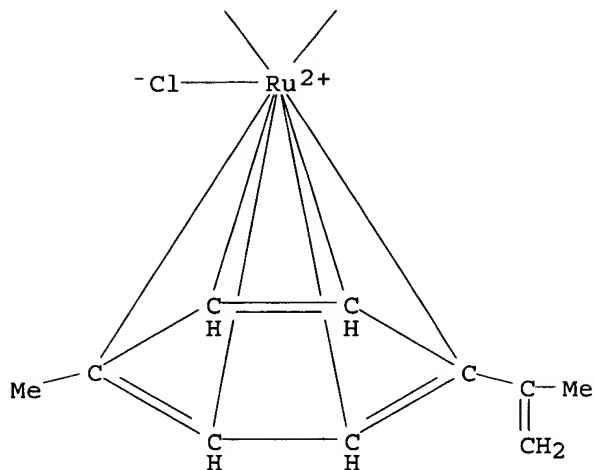
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E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

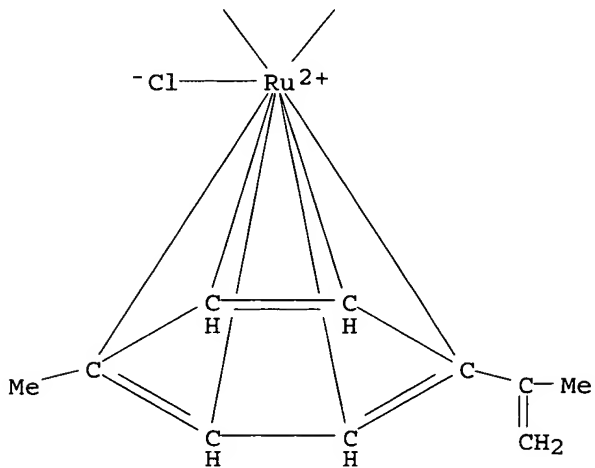
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E

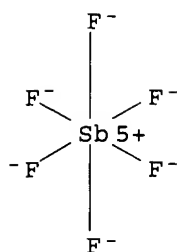
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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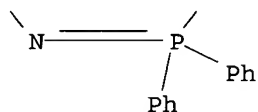


H: CM 1

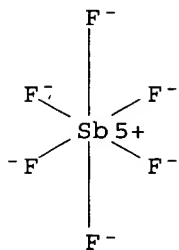
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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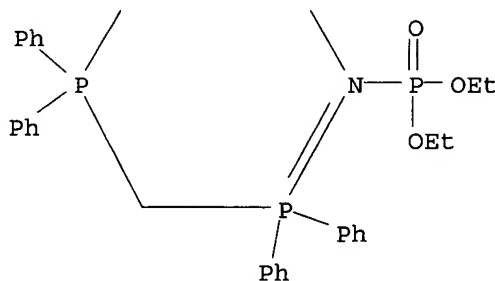
H: CM 2



I: CM 1

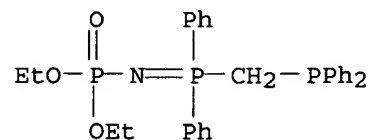
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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I: CM 2

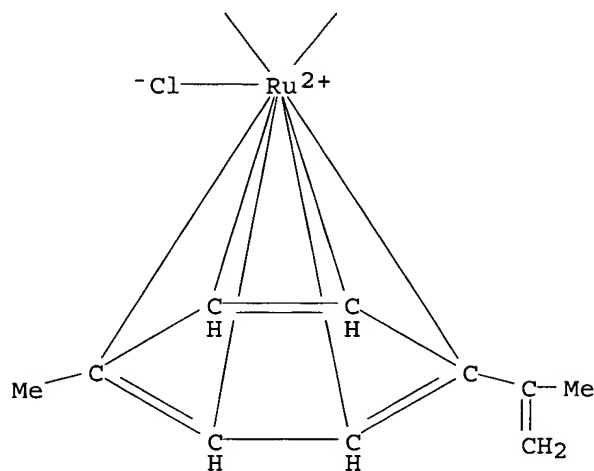
START NEXT REACTION SEQUENCE



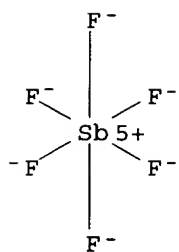
4 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

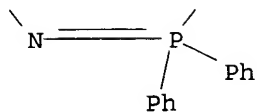


H: CM 1

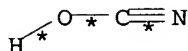
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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H: CM 2



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

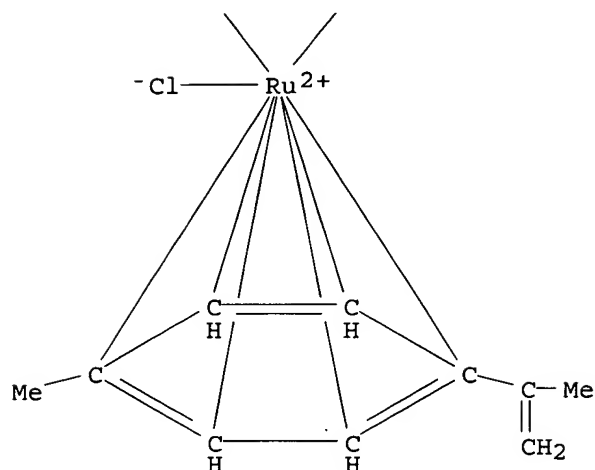
RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(119) OF 151 COMPOSED OF REACTION SEQUENCE RX(1), RX(4), RX(12)
 AND REACTION SEQUENCE RX(2), RX(5), RX(12)

...A + B + 3 E ==> H + I...
 ... C + E + H + 4 W ==> 2 X

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

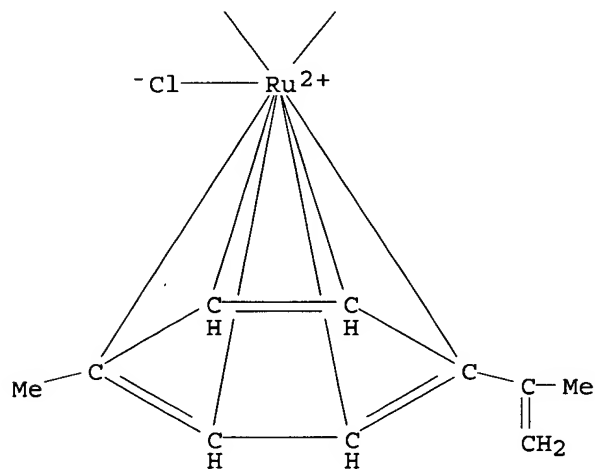
PAGE 2-A



E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

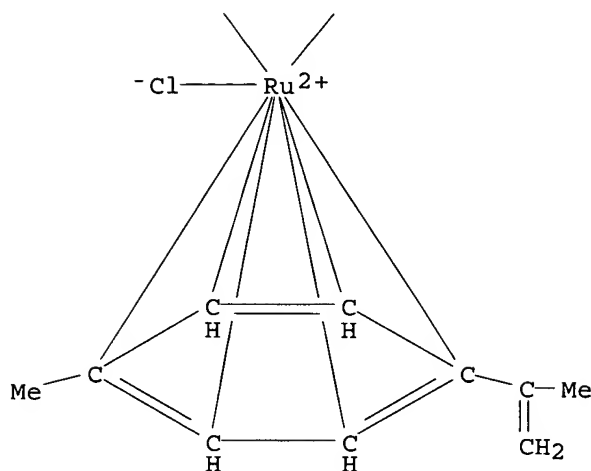
PAGE 2-A



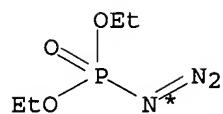
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

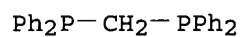
PAGE 2-A



E

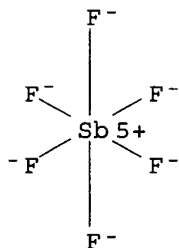


A



B

3
STEPS
→

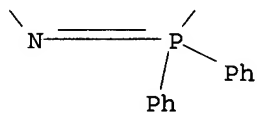


H: CM 1

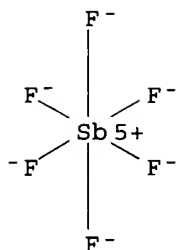
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



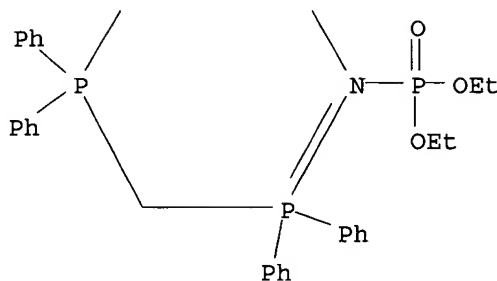
H: CM 2



I: CM 1

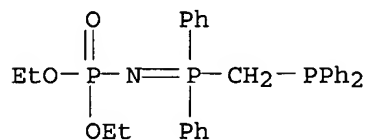
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



I: CM 2

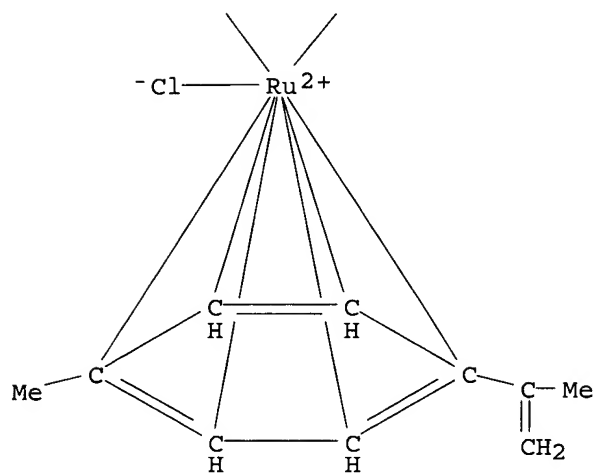
START NEXT REACTION SEQUENCE



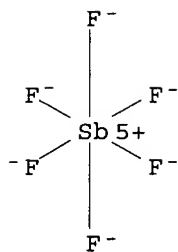
C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

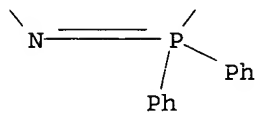


H: CM 1

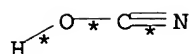
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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H: CM 2



● Na

3

STEPS

4 W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

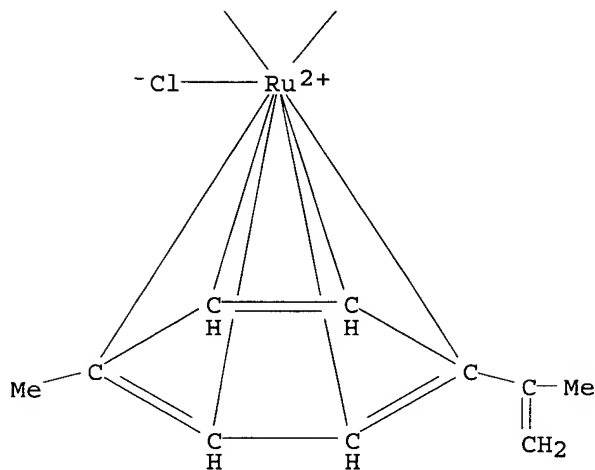
RX(123) OF 151 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(12)
 AND REACTION SEQUENCE RX(2), RX(5), RX(12)

...2 C + 2 E ==> H + I...

... C + E + H + 4 W ==> 2 X

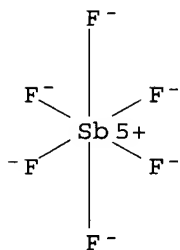
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

3
STEPS
→

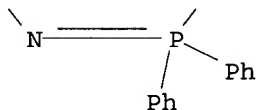


H: CM 1

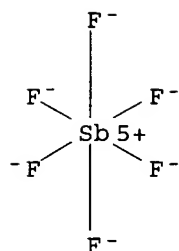
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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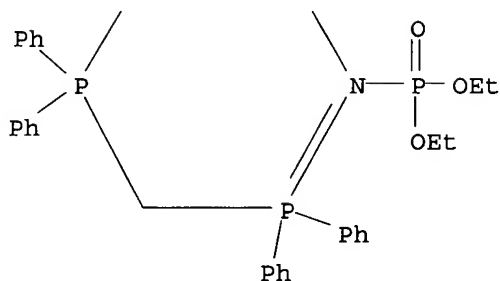
H: CM 2



I: CM 1

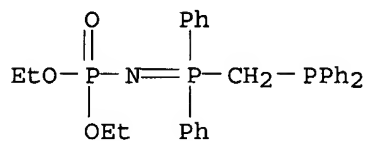
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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I: CM 2

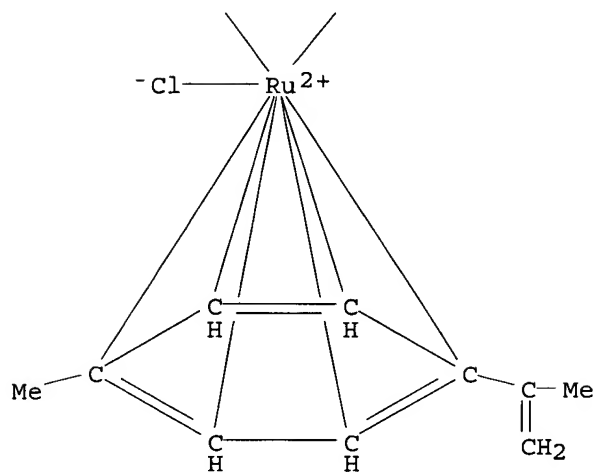
START NEXT REACTION SEQUENCE



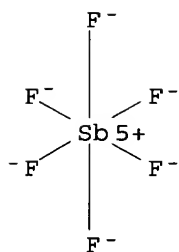
3 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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2 E

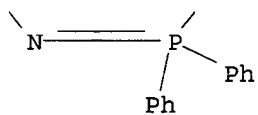


H: CM 1

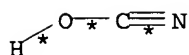
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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H: CM 2



● Na

3

STEPS

4 W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE 85% overall, in dark

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

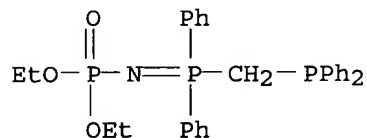
RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(127) OF 151 COMPOSED OF REACTION SEQUENCE RX(4), RX(12)
 AND REACTION SEQUENCE RX(1), RX(2), RX(5), RX(12)

...3 C + 3 E ==> H + I...

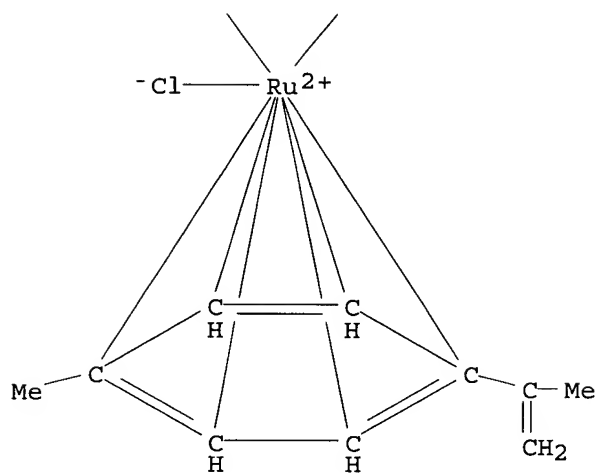
...2 A + 2 B + E + H + 4 W ==> 2 X



3 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

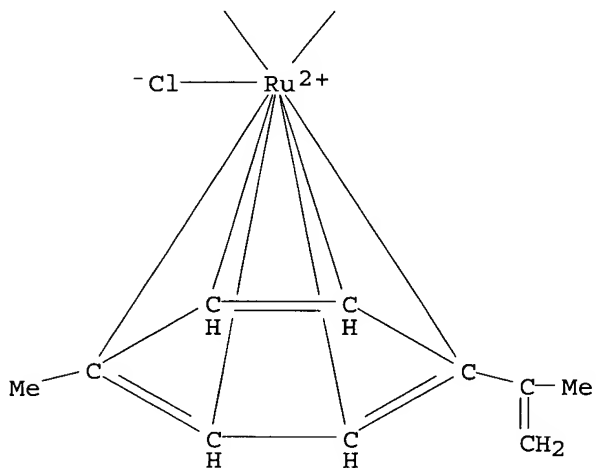
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E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

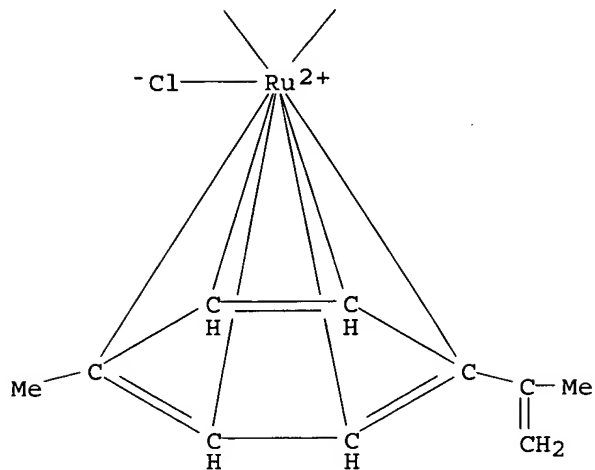
PAGE 2-A



E

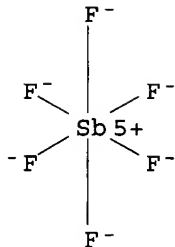
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

4
STEPS
→

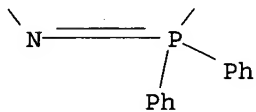


H: CM 1

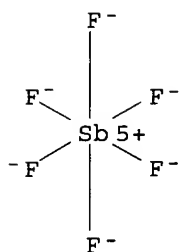
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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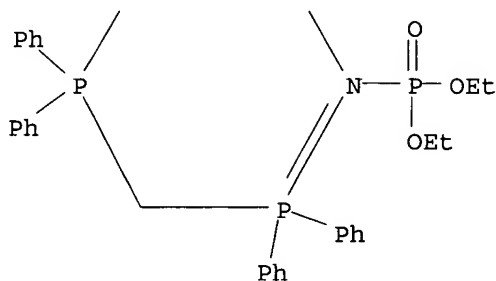
H: CM 2



I: CM 1

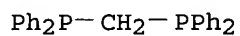
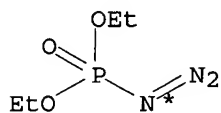
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



I: CM 2

START NEXT REACTION SEQUENCE

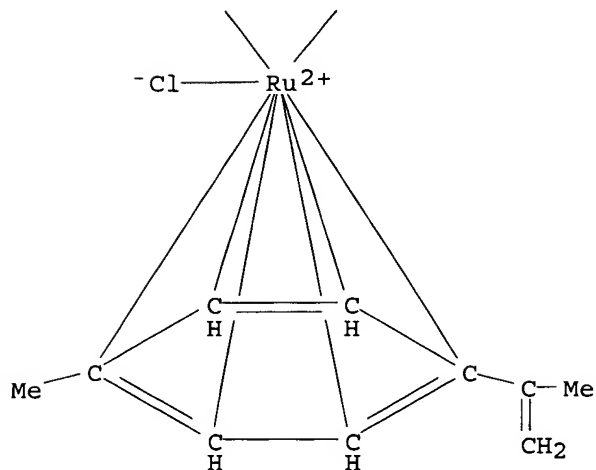


2 A

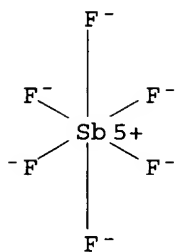
2 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

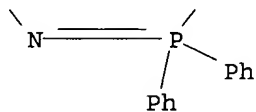


H: CM 1

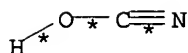
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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H: CM 2



● Na

4

STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF6
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark, 82% overall

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

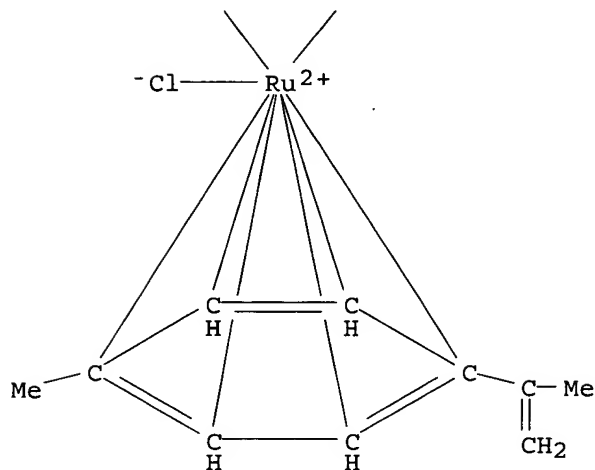
RX(131) OF 151 COMPOSED OF REACTION SEQUENCE RX(1), RX(4), RX(12)
 AND REACTION SEQUENCE RX(1), RX(2), RX(5), RX(12)

...2 A + 2 B + 3 E ==> H + I...

...A + B + E + H + 4 W ==> 2 X

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

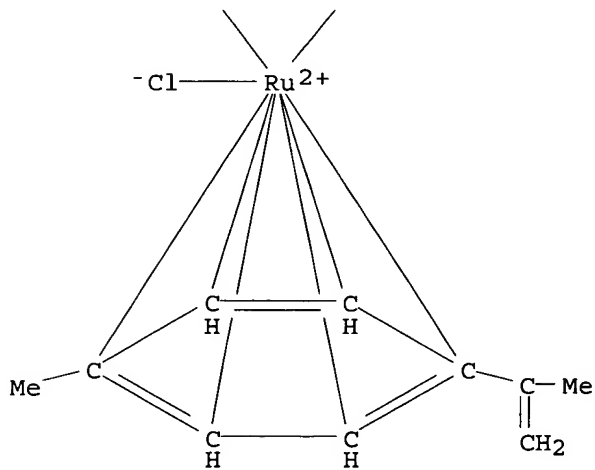
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E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

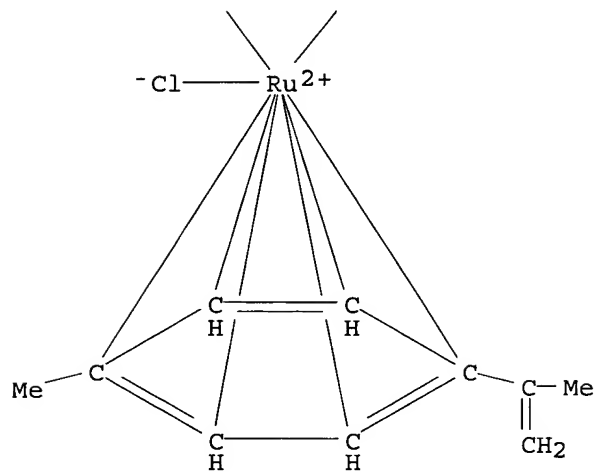
PAGE 2-A



E

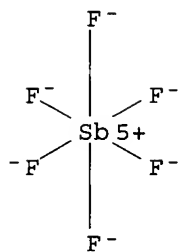
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

4
STEPS
→

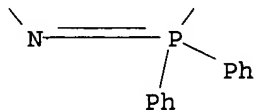


H: CM 1

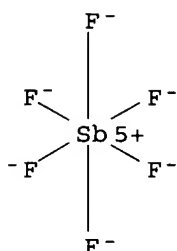
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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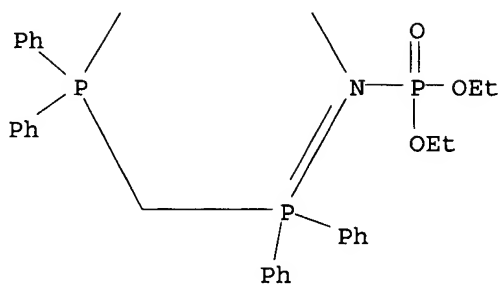
H: CM 2



I: CM 1

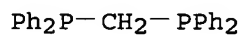
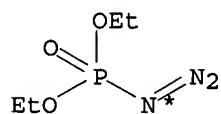
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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I: CM 2

START NEXT REACTION SEQUENCE

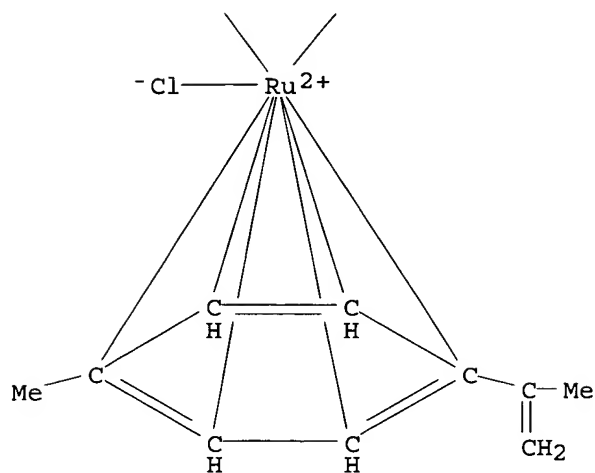


3 A

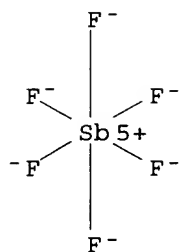
3 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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E

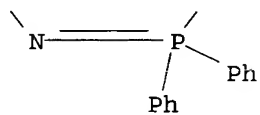


H: CM 1

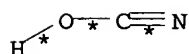
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



H: CM 2



● Na

4

STEPS

4 W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(4) RCT C 540518-26-1, E 135585-10-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark, 82% overall

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

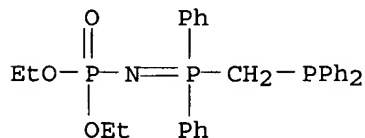
RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(135) OF 151 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(12)
 AND REACTION SEQUENCE RX(1), RX(2), RX(5), RX(12)

...2 C + 2 E ==> H + I...

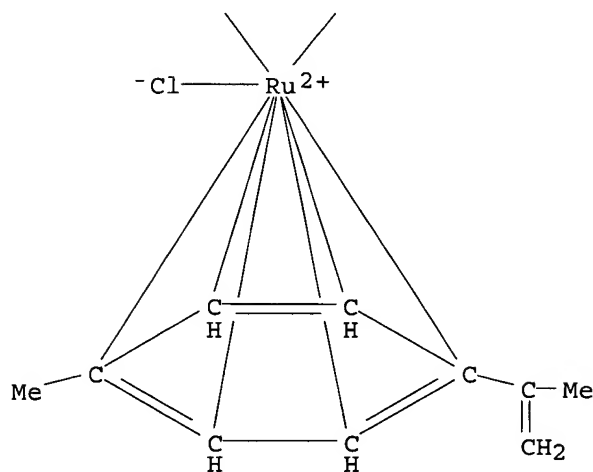
...2 A + 2 B + E + H + 4 W ==> 2 X



2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

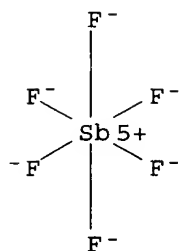
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E

4

STEPS
→

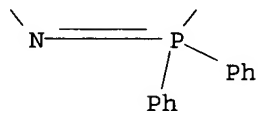


H: CM 1

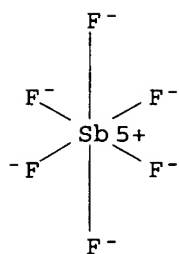
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



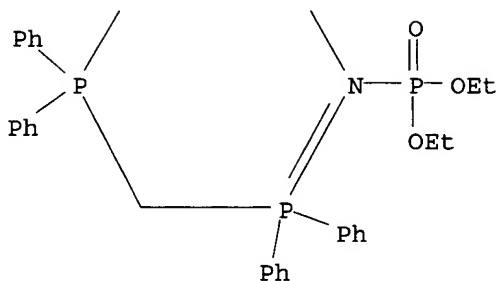
H: CM 2



I: CM 1

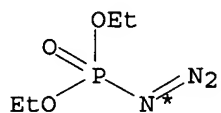
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

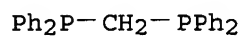


I: CM 2

START NEXT REACTION SEQUENCE



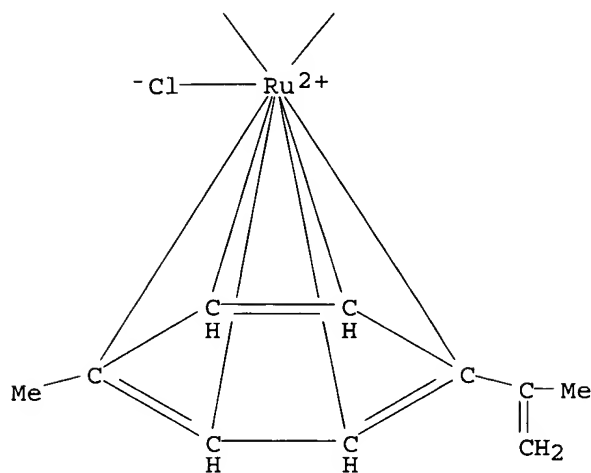
2 A



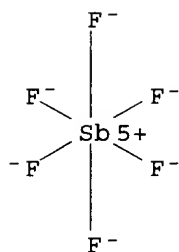
2 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E

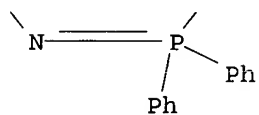


H: CM 1

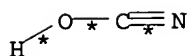
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



H: CM 2



● Na

4

STEPS

4 W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE 85% overall, in dark

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

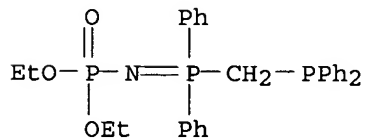
RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(139) OF 151 COMPOSED OF REACTION SEQUENCE RX(2), RX(5), RX(12)
 AND REACTION SEQUENCE RX(3), RX(12)

...2 C + 2 E ==> I...

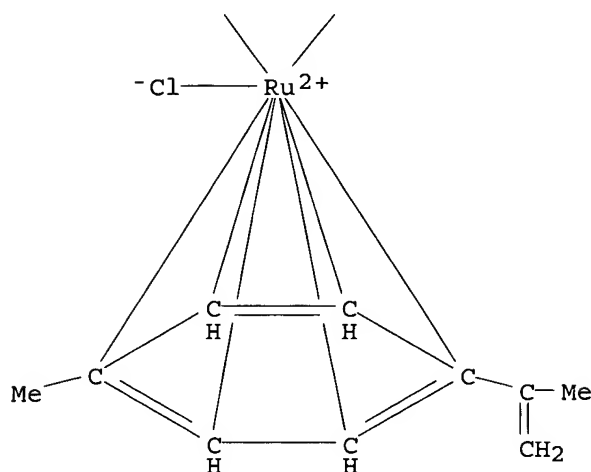
...2 F + 4 W ==> 2 X



2 C

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

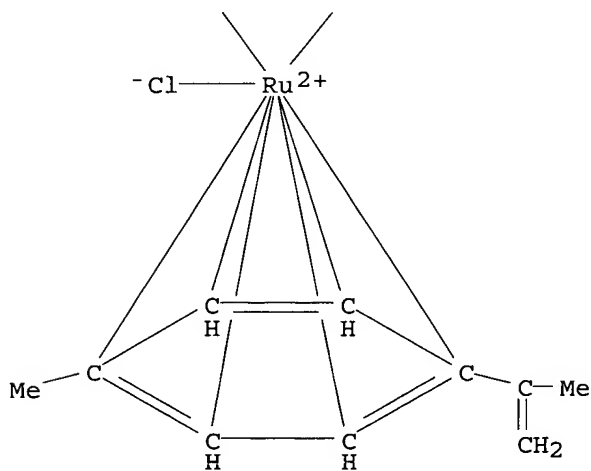
PAGE 2-A



E

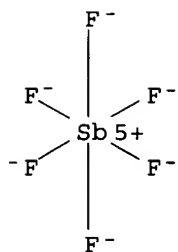
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



E

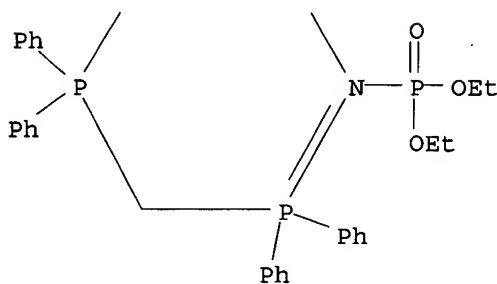
2
STEPS
→



I: CM 1

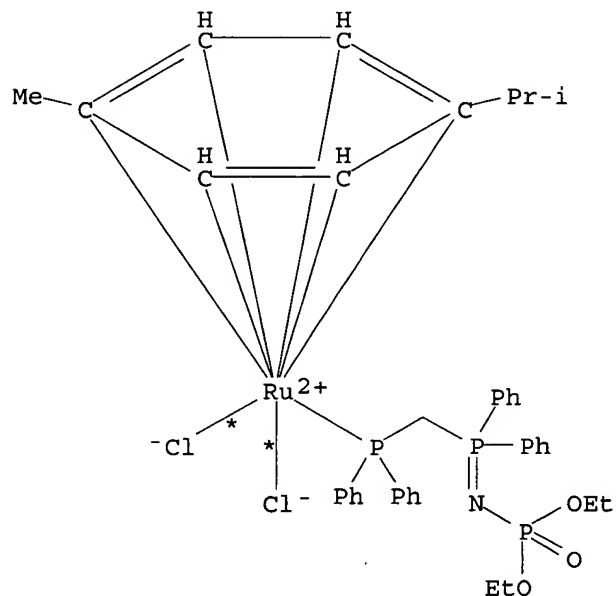
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



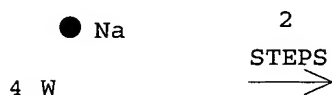
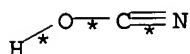
I: CM 2

START NEXT REACTION SEQUENCE



F

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

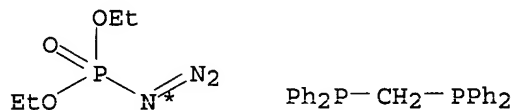
RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(143) OF 151 COMPOSED OF REACTION SEQUENCE RX(1), RX(2), RX(5), RX(12)
 AND REACTION SEQUENCE RX(3), RX(12)

...2 A + 2 B + 2 E ==> I...

...2 F + 4 W ==> 2 X

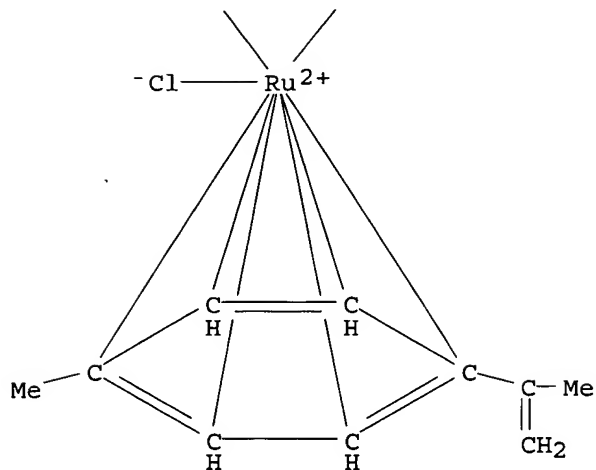


2 A

2 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

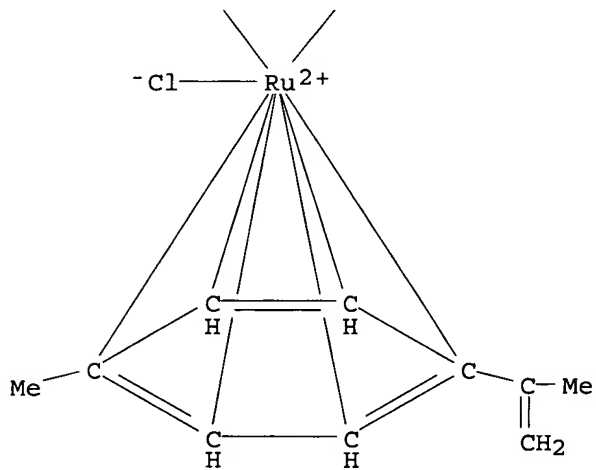
PAGE 2-A



E

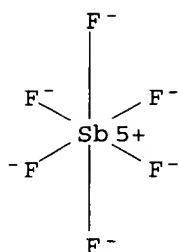
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



E

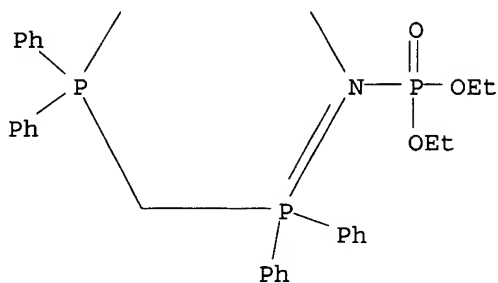
2
STEPS
→



I: CM 1

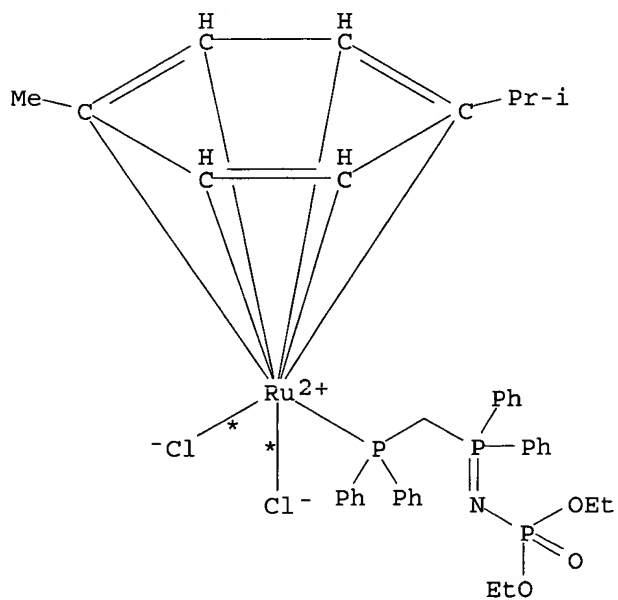
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



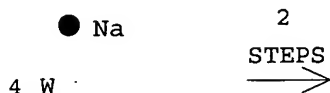
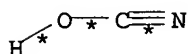
I: CM 2

START NEXT REACTION SEQUENCE



F

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 1516-68-3, B 2071-20-7
 PRO C 540518-26-1
 SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH₂Cl₂

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE in dark

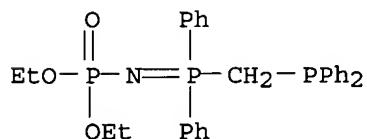
RX(3) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF₆
 PRO H 540518-31-8, I 540518-34-1
 SOL 75-09-2 CH₂Cl₂
 NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
 PRO X 540518-52-3
 SOL 67-56-1 MeOH

RX(147) OF 151 COMPOSED OF REACTION SEQUENCE RX(2), RX(5), RX(12)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(12)

...3 C + 3 E ==> I...

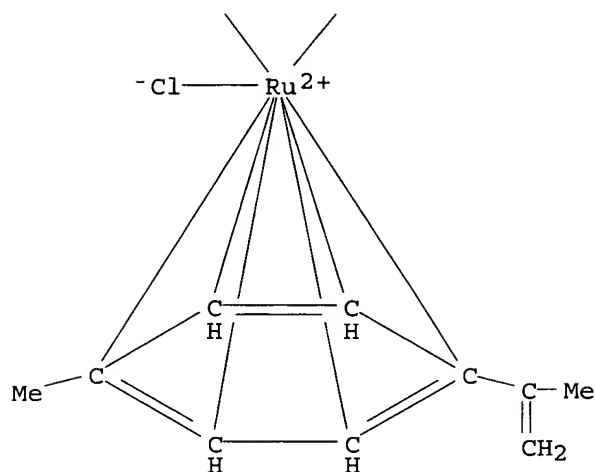
...A + B + E + 4 W ==> 2 X



3 C

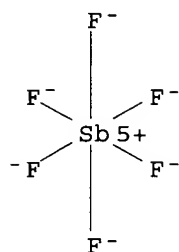
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E

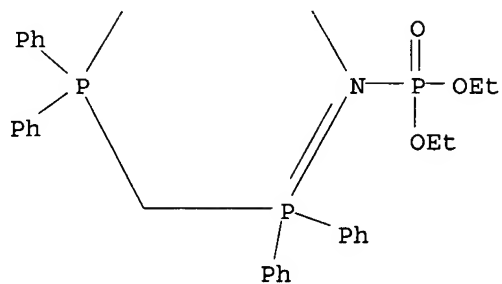
4
STEPS
→



I: CM 1

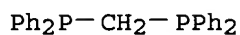
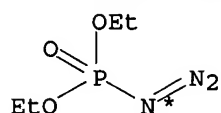
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



I: CM 2

START NEXT REACTION SEQUENCE

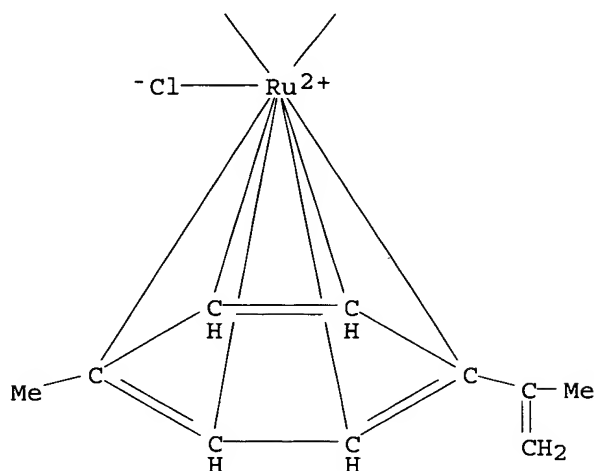


A

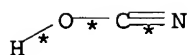
B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E



● Na

4

STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 540518-26-1, E 135585-10-3
 PRO F 540518-28-3
 SOL 75-09-2 CH2Cl2

RX(5) RCT F 540518-28-3
 RGT J 26042-64-8 AgSbF6
 PRO K 540518-37-4, I 540518-34-1
 SOL 75-09-2 CH2Cl2
 NTE in dark

RX(1) RCT A 1516-68-3, B 2071-20-7
PRO C 540518-26-1
SOL 109-99-9 THF

RX(2) RCT C 540518-26-1, E 135585-10-3
PRO F 540518-28-3
SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
RGT J 26042-64-8 AgSbF₆
PRO H 540518-31-8, I 540518-34-1
SOL 75-09-2 CH₂Cl₂
NTE 85% overall, in dark

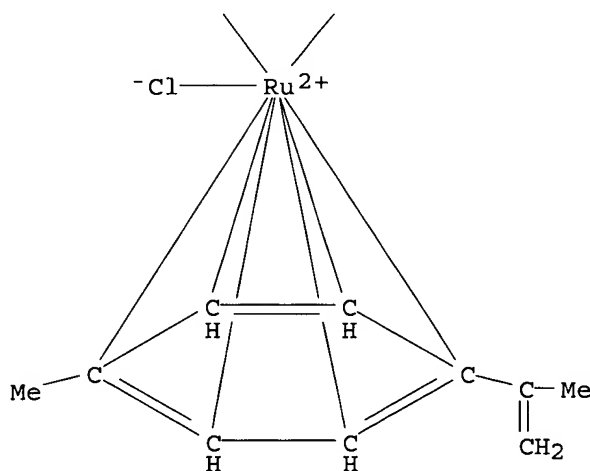
RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
PRO X 540518-52-3
SOL 67-56-1 MeOH

RX(151) OF 151 COMPOSED OF REACTION SEQUENCE RX(1), RX(2), RX(5), RX(12)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(12)

...3 A + 3 B + 3 E ==> I...
...A + B + E + 4 W ==> 2 X

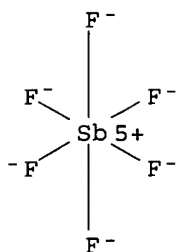
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E

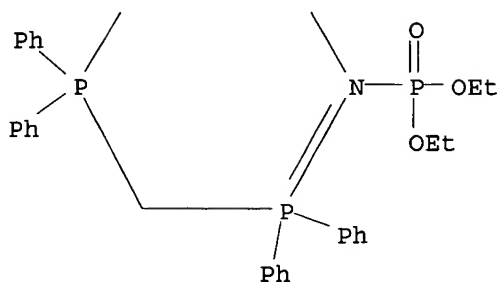
4
STEPS
→



I: CM 1

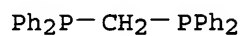
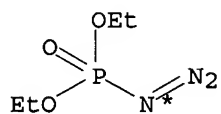
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



I: CM 2

START NEXT REACTION SEQUENCE

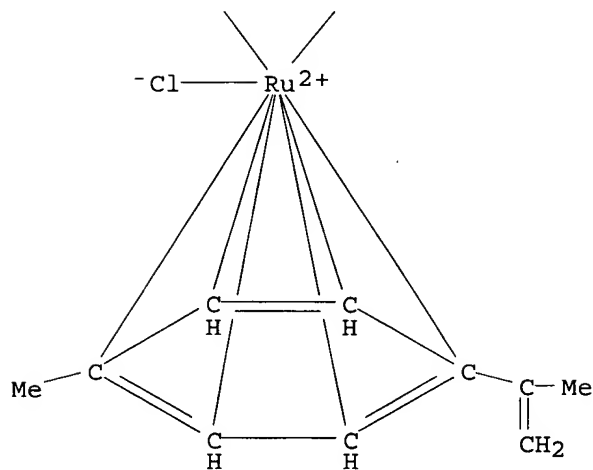


4 A

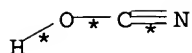
4 B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



2 E



● Na

4

STEPS

4 W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1)	RCT	A 1516-68-3, B 2071-20-7
	PRO	C 540518-26-1
	SOL	109-99-9 THF
RX(2)	RCT	C 540518-26-1, E 135585-10-3
	PRO	F 540518-28-3
	SOL	75-09-2 CH ₂ Cl ₂
RX(5)	RCT	F 540518-28-3
	RGT	J 26042-64-8 AgSbF ₆
	PRO	K 540518-37-4, I 540518-34-1
	SOL	75-09-2 CH ₂ Cl ₂
	NTE	in dark
RX(1)	RCT	A 1516-68-3, B 2071-20-7
	PRO	C 540518-26-1
	SOL	109-99-9 THF
RX(2)	RCT	C 540518-26-1, E 135585-10-3
	PRO	F 540518-28-3

SOL 75-09-2 CH₂Cl₂

RX(3) RCT F 540518-28-3
RGT J 26042-64-8 AgSbF₆
PRO H 540518-31-8, I 540518-34-1
SOL 75-09-2 CH₂Cl₂
NTE 85% overall, in dark

RX(12) RCT H 540518-31-8, I 540518-34-1, W 917-61-3
PRO X 540518-52-3
SOL 67-56-1 MeOH

L49 ANSWER 3 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 138:89485 CASREACT

TITLE: Synthesis and studies of 6,6'-BINAP derivatives for the heterogeneous asymmetric hydrogenation of methyl acetoacetate

AUTHOR(S): Saluzzo, Christine; Lamouille, Thierry; Le Guyader, Frederic; Lemaire, Marc

CORPORATE SOURCE: CPE, UMR 5622, Laboratoire de Catalyse et Synthese Organique, Universite Claude Bernard, Villeurbanne, 69622, Fr.

SOURCE: Tetrahedron: Asymmetry (2002), 13(11), 1141-1146

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

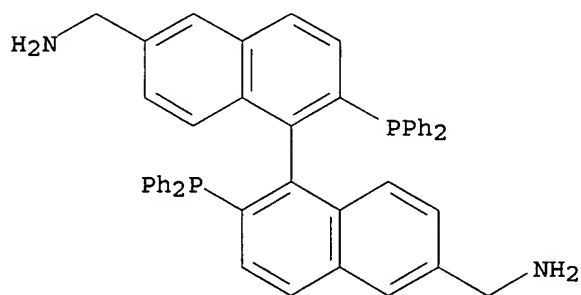
DOCUMENT TYPE: Journal

LANGUAGE: English

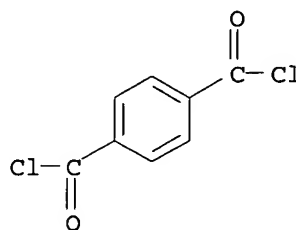
AB New BINAP derivs. (polyamide, polyureas or ureas) were synthesized and employed in the ruthenium-catalyzed asym. heterogeneous hydrogenation of Me acetoacetate. Enantiomeric excesses in the range 48-100% were observed. Furthermore, the most efficient have been recovered and the recycled catalysts were shown to maintain their efficiency in subsequent reactions.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

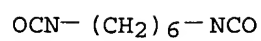
RX(4) OF 7 A + K ==> L



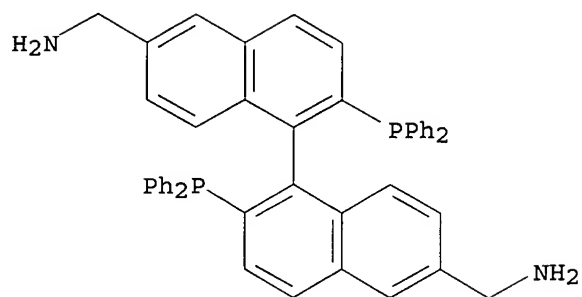
A: CM 1



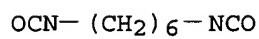
A: CM 2



K

(4) \longrightarrow 

L: CM 1
YIELD 96%



L: CM 2

YIELD 96%

RX(4) RCT A 291772-79-7, K 822-06-0

STAGE(1)

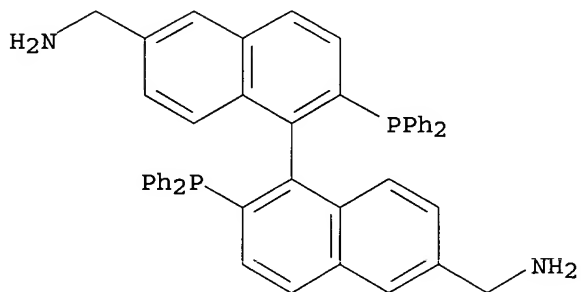
SOL 75-09-2 CH2Cl2

STAGE(2)

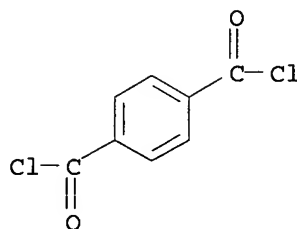
SOL 67-63-0 Me2CHOH

PRO L 291772-80-0

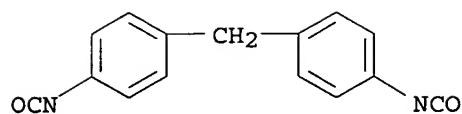
RX(5) OF 7 A + M ==> N



A: CM 1

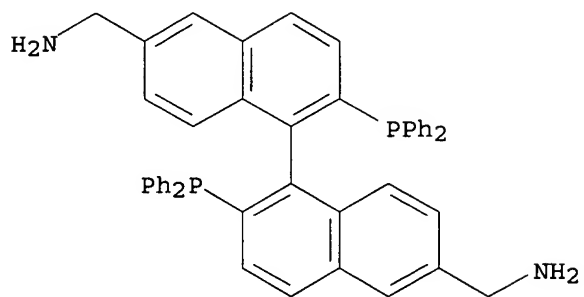
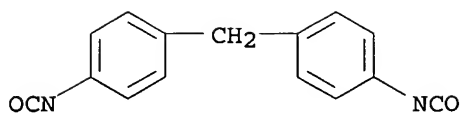


A: CM 2



M

(5)

N: CM 1
YIELD 76%N: CM 2
YIELD 76%

RX(5) RCT A 291772-79-7, M 101-68-8

STAGE(1)

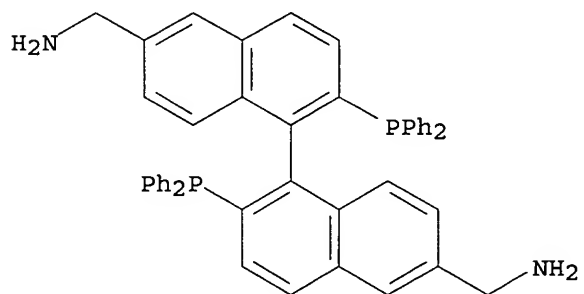
SOL 75-09-2 CH₂Cl₂

STAGE(2)

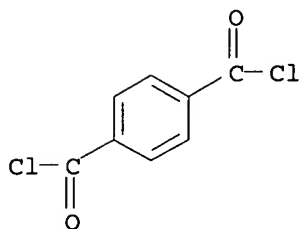
SOL 67-63-0 Me₂CHOH

PRO N 479672-81-6

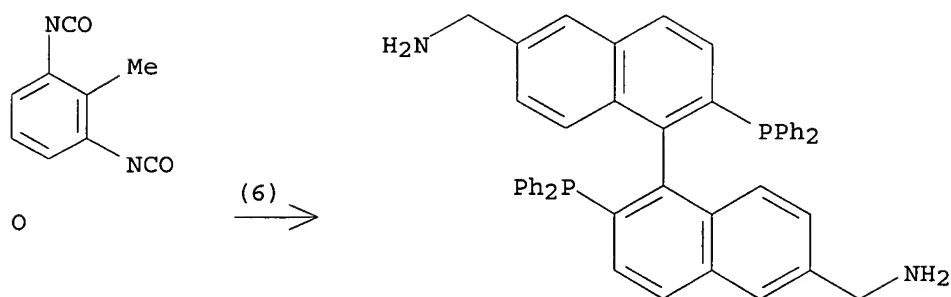
RX(6) OF 7 A + O ==> P



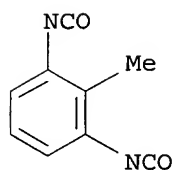
A: CM 1



A: CM 2



P: CM 1
YIELD 93%



P: CM 2
YIELD 93%

RX(6) RCT A 291772-79-7, O 91-08-7

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

SOL 67-63-0 Me2CHOH

PRO P 263173-51-9

L49 ANSWER 4 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 137:140604 CASREACT

TITLE: Ruthenium(II) and ruthenium(IV) complexes containing hemilabile heterodifunctional iminophosphorane-phosphine ligands Ph₂PCH₂P(:NR)Ph₂

AUTHOR(S): Cadierno, Victorio; Diez, Josefina; Garcia-Garrido, Sergio E.; Garcia-Granda, Santiago; Gimeno, Jose

CORPORATE SOURCE: Departamento de Quimica Organica e Inorganica, Instituto Universitario de Quimica Organometalica 'Enrique Moles' (Unidad Asociada al C.S.I.C.), Universidad de Oviedo, Oviedo, E-33071, Spain

SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (7), 1465-1472

CODEN: JCSDA; ISSN: 1472-7773

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

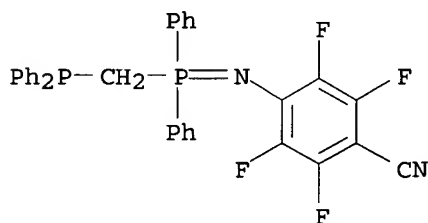
AB The dimeric complex [{Ru(η⁶-p-cymene)(μ-Cl)Cl}₂] reacts with iminophosphorane-phosphine ligands Ph₂PCH₂P(:NR)Ph₂ (R = SiMe₃ 1, p-C₆F₄CN

2, p-C5F4N 3), in dichloromethane at room temperature, to afford the neutral derivs. $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}_2\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}]$ (R = SiMe₃ 4, p-C6F4CN 5, p-C5F4N 6). Treatment of 4-6 with NaPF₆ in methanol allows the preparation of cationic species $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}\{\kappa^2\text{-P,N-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}][\text{PF}_6]$ (R = H 7, p-C6F4CN 8, p-C5F4N 9). While complexes 8 and 9 react with anionic ligands yielding neutral derivs. $[\text{Ru}(\eta^6\text{-p-cymene})\text{X}_2\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}]$ (R = p-C6F4CN, X = Br 10a, I 10b, N₃ 10c, CN 10d, NCO 10e; R = p-C5F4N, X = Br 11a, I 11b, N₃ 11c, CN 11d, NCO 11e), cationic species $[\text{Ru}(\eta^6\text{-p-cymene})\text{X}\{\kappa^2\text{-P,N-Ph}_2\text{PCH}_2\text{P}(\text{:NH})\text{Ph}_2\}][\text{PF}_6]$ (X = Br 12a, I 12b, N₃ 12c, CN 12d, NCO 12e) are exclusively formed starting from 7. Complexes 8 and 9 also react with neutral ligands such as phosphines, pyridine, acetonitrile or isocyanides affording compds. $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}(\text{PR}_3)\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}][\text{PF}_6]$ (R = p-C6F4CN, PR₃ = PMe₃ 13a, PMe₂Ph 13b, PMePh₂ 13c, PPh₃ 13d; R = p-C5F4N, PR₃ = PMe₃ 14a, PMe₂Ph 14b, PMePh₂ 14c, PPh₃ 14d), $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}(\text{py})\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}][\text{PF}_6]$ (R = p-C6F4CN 15; R = p-C5F4N 16), $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}(\text{N.tplbond.CMe})\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}][\text{PF}_6]$ (R = p-C6F4CN 17; R = p-C5F4N 18) and $[\text{Ru}(\eta^6\text{-p-cymene})\text{Cl}(\text{CNR}')\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}][\text{PF}_6]$ (R = p-C6F4CN, R' = Cy 19a, 2,6-C6H3Me₂ 19b; R = p-C5F4N, R' = Cy 20a, 2,6-C6H3Me₂ 20b), resp. The synthesis of complexes $[\text{Ru}(\eta^3:\eta^3\text{-C}_{10}\text{H}_{16})\text{Cl}_2\{\kappa^1\text{-P-Ph}_2\text{PCH}_2\text{P}(\text{:NR})\text{Ph}_2\}]$ (R = SiMe₃ 21, p-C6F4CN 22, p-C5F4N 23) and $[\text{Ru}(\eta^3:\eta^3\text{-C}_{10}\text{H}_{16})\text{Cl}\{\kappa^2\text{-P,N-Ph}_2\text{PCH}_2\text{P}(\text{:NH})\text{Ph}_2\}][\text{BF}_4]$ 24 starting from the bis(allyl)-ruthenium(IV) dimer $[\{\text{Ru}(\eta^3:\eta^3\text{-C}_{10}\text{H}_{16})(\mu\text{-Cl})\text{Cl}\}_2]$ and ligands 1-3 is also reported. The crystal structure of 10e·CH₂Cl₂ is reported.

REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(83) OF 102 COMPOSED OF RX(2), RX(5), RX(11)

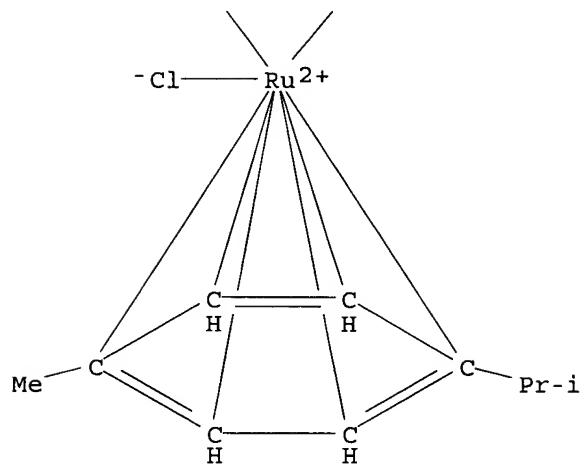
RX(83) E + B + 2 V ==> W



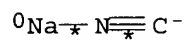
E

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



B



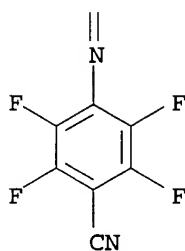
3

2 V

 STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



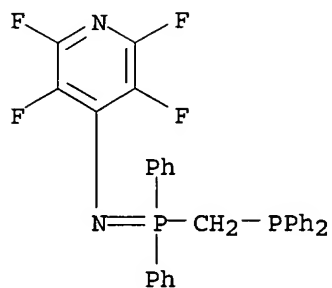
W

YIELD 71%

RX(2)	RCT	E 121524-38-7, B 52462-29-0
	PRO	F 444940-44-7
	SOL	75-09-2 CH2Cl2
RX(5)	RCT	F 444940-44-7
	RGT	J 21324-39-0 NaPF6
	PRO	L 444940-49-2
	SOL	67-56-1 MeOH
RX(11)	RCT	L 444940-49-2, V 70152-47-5

PRO W 444940-56-1
SOL 67-56-1 MeOH

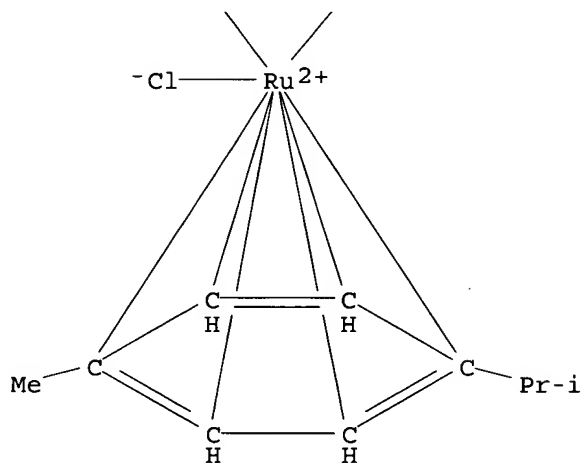
RX(95) OF 102 COMPOSED OF RX(3), RX(6), RX(16)
RX(95) G + B + 2 V ==> AB



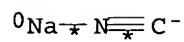
G

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



B

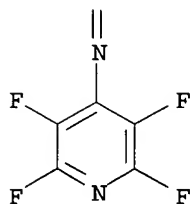


2 V



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



AB

YIELD 73%

RX(3) RCT G 121498-14-4, B 52462-29-0
PRO H 444940-45-8
SOL 75-09-2 CH₂Cl₂

RX(6) RCT H 444940-45-8
RGT J 21324-39-0 NaPF₆
PRO M 444940-51-6
SOL 67-56-1 MeOH

RX(16) RCT M 444940-51-6, V 70152-47-5
PRO AB 444940-61-8
SOL 67-56-1 MeOH

L49 ANSWER 5 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 135:273066 CASREACT

TITLE: Cleavage of the dimeric cyclopalladated
[Pd(N,C-dmba)(μ-X)]₂, (dmba = N,N-
dimethylbenzylamine; X = SCN and NCO) by diphosphines.
Palladium(II) compounds with distinct structures in
the solid-state and in solution

AUTHOR(S): Ananias, Sandra R.; Mauro, Antonio E.; De Lucca Neto,
Vicente A.

CORPORATE SOURCE: Instituto de Quimica de Araraquara, UNESP, Araraquara,
14801-970, Brazil

SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands)
(2001), 26(4-5), 570-573
CODEN: TMCHDN; ISSN: 0340-4285

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

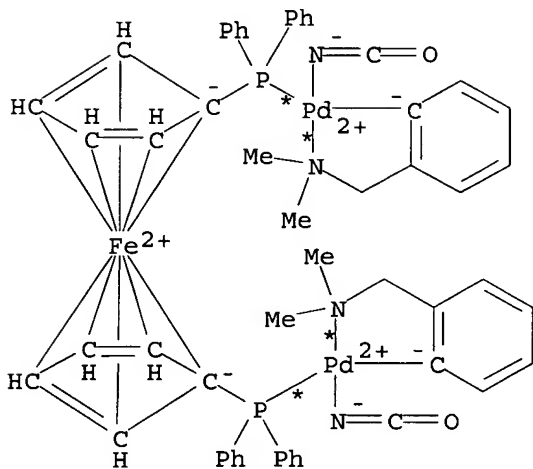
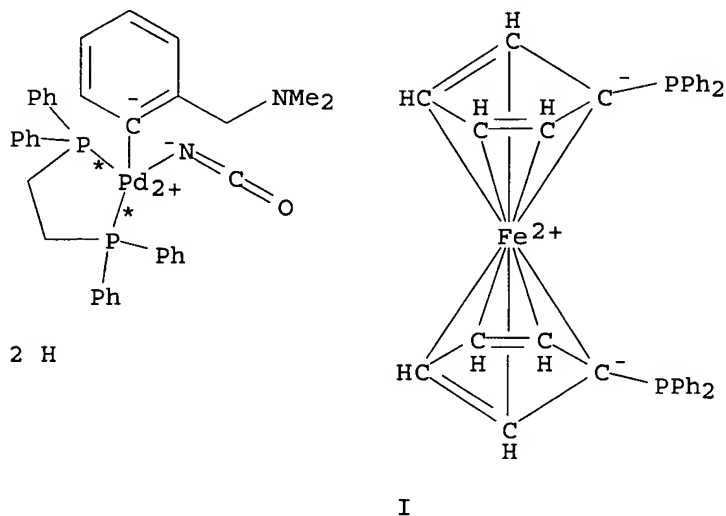
AB The reactions of the pseudohalide-bridged dimer [Pd(N,C-dmba)(μ-SCN)]₂ (1) (dmba = N,N-dimethylbenzylamine) with cis-Ph₂PCH:CHPh₂ (cis-dppet) (1:1 molar ratio) and of [Pd(N,C-dmba)(μ-NCO)]₂ (2) with Ph₂PCH₂CH₂PPh₂ (dppe) (1:2 molar ratio) gave mononuclear [Pd(C-dmba)(SCN)(cis-dppet)]·H₂O (1a) and [Pd(C-dmba)(NCO)(dppe)] (2a), resp., with the diphosphines acting as chelating ligands. Reaction of (2) with Fe(C₅H₄PPh₂)₂ (dppf) (1:1 molar ratio) yielded [{Pd(N,C-dmba)(NCO)}₂(μ-dppf)] (2b), a bimetallic species containing two Pd atoms bridged by the diphosphine, whereas reaction in a 1:2 molar ratio gave the mononuclear [Pd(N,C-dmba)(dppf)] [NCO]·CH₂Cl₂ (2c), with the diphosphine acting as a chelating ligand. The compds. were characterized by elemental anal., IR, ³¹P{¹H}, ¹³C- and ¹H-NMR spectroscopies. Conductivity measurements together

with spectroscopic data showed that (1a) and (2a) do not have the same

structure in the solid state and in MeCl solution, whereas for compds. (2b) and (2c) no structural changes were observed when the solids were dissolved in MeCl.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

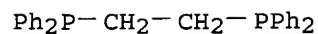
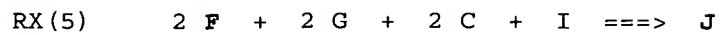
RX(3) OF 6 ...2 H + I ==> J



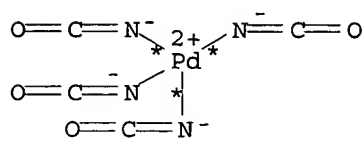
J
YIELD 80%

RX(3) RCT H 362624-31-5, I 12150-46-8
PRO J 362624-32-6
SOL 75-09-2 CH2Cl2

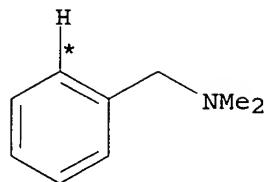
RX(5) OF 6 COMPOSED OF RX(2), RX(3)



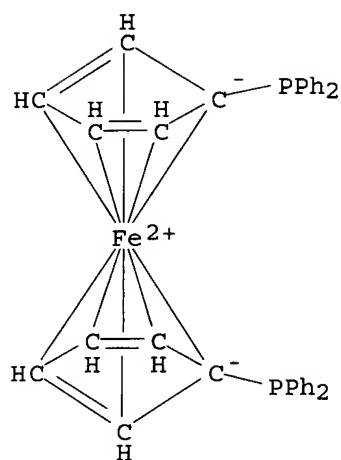
2 F



2 G

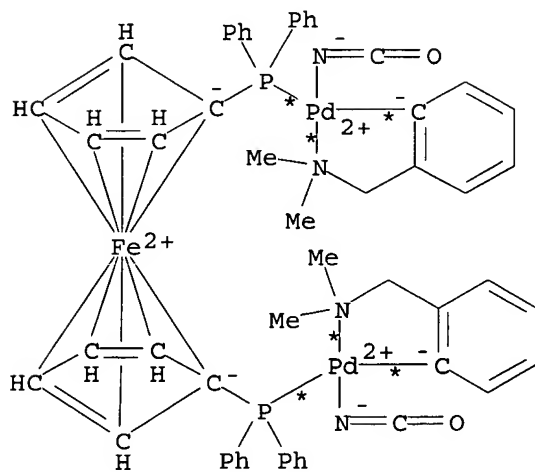


2 C



I

2
STEPS
→



J

YIELD 80%

RX(2) RCT F 1663-45-2, G 45073-61-8, C 103-83-3
PRO H 362624-31-5
SOL 67-64-1 Me2CO

RX(3) RCT H 362624-31-5, I 12150-46-8
PRO J 362624-32-6
SOL 75-09-2 CH2Cl2

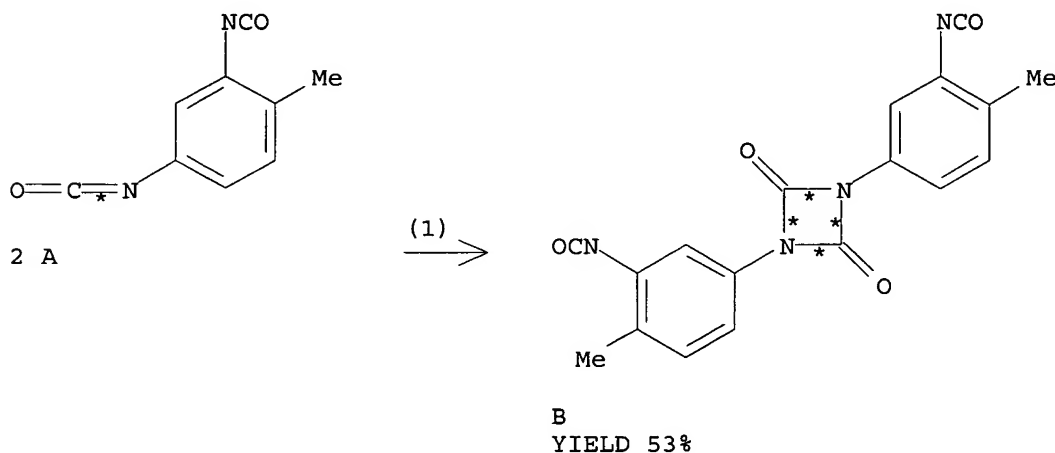
L49 ANSWER 6 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 131:310576 CASREACT
TITLE: Preparation, characterization, and selective reactions of novel [1,3]diazetidines-2,4-diones (uretdiones). A new route to generate asymmetric substituted tolylene diisocyanate derivatives
AUTHOR(S): Risch, Nikolaus; Westerwelle, Ulrich; Kiene, Jurgen; Keuper, Ralf
CORPORATE SOURCE: Fachbereich Chemie Chemietechnik, Univ.-GH Paderborn, Paderborn, D-33098, Germany
SOURCE: Journal fuer Praktische Chemie (Weinheim, Germany) (1999), 341(7), 616-619
CODEN: JPCHF4; ISSN: 1436-9966
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The selective cyclodimerization of 2,4-(OCN)2C6H3Me yields a [1,3]diazetidines-2,4-dione. On this basis, a new method for the selective transformation of the NCO-groups of asym. substituted diisocyanates is described. The reaction with different nucleophiles yields carbamates and ureas.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 16 2 A ==> B...



RX(1) RCT A 584-84-9
RGT C 603-35-0 PPh3
PRO B 3320-33-0
SOL 108-88-3 PhMe

L49 ANSWER 7 OF 7 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 112:98729 CASREACT

TITLE: Organometallic Lewis acids. XXXVIII. Monomeric and bridged pentacarbonyldiphosphinerhenium complexes and their reactions with nucleophiles

AUTHOR(S): Steil, Peter; Nagel, Ulrich; Beck, Wolfgang

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.

SOURCE: Journal of Organometallic Chemistry (1989), 366(3), 313-31

CODEN: JORCAI; ISSN: 0022-328X

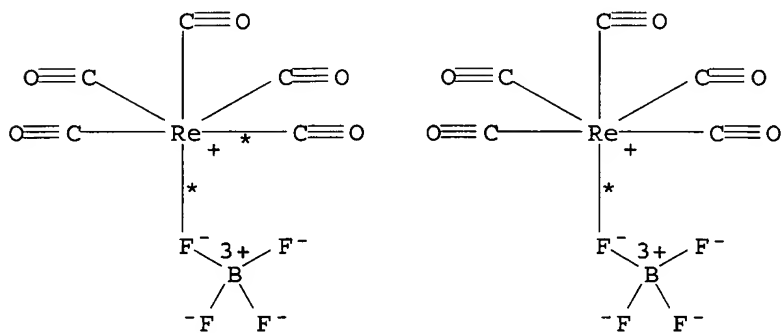
DOCUMENT TYPE: Journal

LANGUAGE: German

AB Pentacarbonyltetrafluorobororhenium, $(OC)_5ReFBF_3$, reacts with diphosphines Ph_2EXEPH_2 ($X = CH_2, CH_2CH_2, NH$; $E = P, As$) to give monomeric and bridged complexes $[(OC)_5ReEPH_2XEPH_2]^+$, $[(OC)_5ReEPH_2XPh_2ERe(CO)_5]^2+$. The crystal structures of $[(OC)_5RePPh_2NHPPH_2]^+$ and $[(OC)_5RePPh_2CH_2CH_2PPh_2Re(CO)_5]^2+$ have been determined by an x-ray diffraction study. In solution the tautomers $[(OC)_5RePPh_2NHPPH_2]^+$ and $[(OC)_5RePPh_2:NP(H)Ph_2]^+$ have been detected by NMR spectroscopy. Attack by hydroxide and methoxide occurs at a carbonyl ligand of these complexes to give hydroxycarbonyl, hydrido and methoxycarbonyl complexes, resp. The azide ion adds to a carbonyl ligand to give the isocyanato complexes $(NCO)(OC)_4ReEPH_2CH_2CH_2EPH_2Re(CO)_4(NCO)$ ($E = P, As$) and $(NCO)(OC)_4RePPh_2NHPPH_2$. The latter complex loses carbon monoxide to give $(OCN)(OC)_3RePPh_2NHPPH_2$, which was characterized by x-ray diffraction.

RX(22) OF 26 COMPOSED OF RX(6), RX(15)

RX(22) 2 A + L ==> AA



A

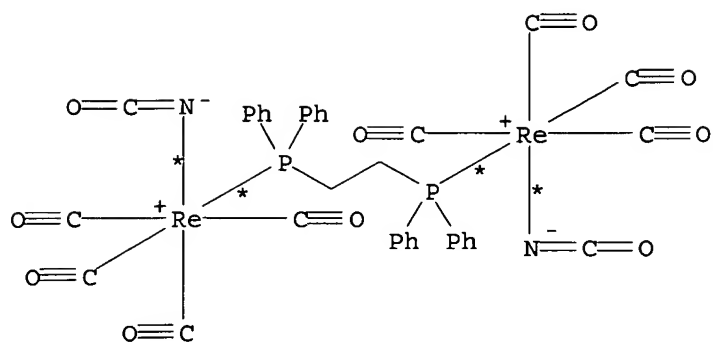
A

Ph₂P-CH₂-CH₂-PPh₂

2

L

STEPS
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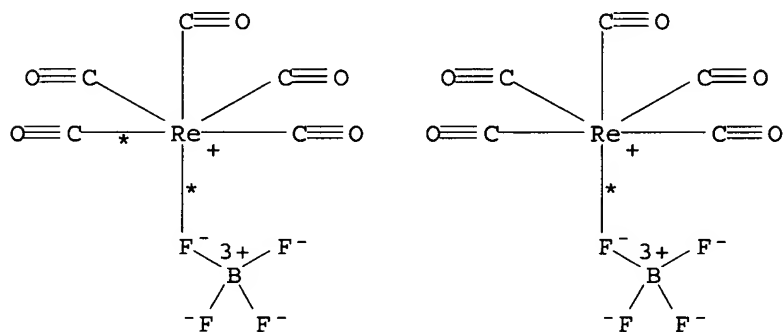
AA

RX(6) RCT A 78670-75-4, L 1663-45-2
 PRO M 125392-31-6
 SOL 75-09-2 CH2Cl2

RX(15) RCT M 125392-31-6
 RGT Y 26628-22-8 NaN3
 PRO AA 125467-56-3
 SOL 67-64-1 Me2CO, 7732-18-5 Water

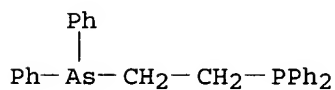
RX(24) OF 26 COMPOSED OF RX(7), RX(16)

RX(24) 2 A + G ==> AB



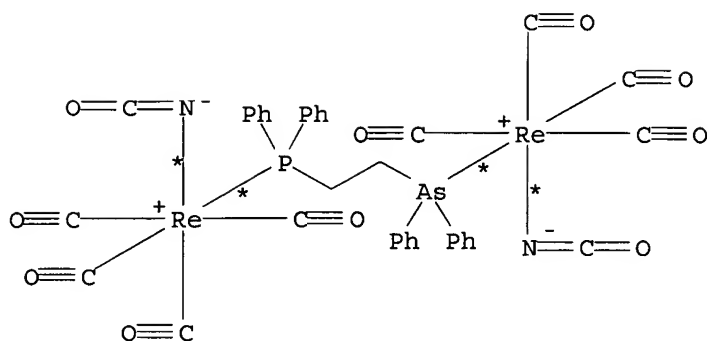
A

A



G

2
 STEPS
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AB

RX (7) RCT A 78670-75-4, G 23582-06-1
 PRO N 125392-33-8
 SOL 75-09-2 CH₂Cl₂

RX (16) RCT N 125392-33-8
 RGT Y 26628-22-8 NaN₃
 PRO AB 125467-57-4
 SOL 67-64-1 Me₂CO, 7732-18-5 Water

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FILE LAST UPDATED: 26 May 2005 (20050526/ED)

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L5 796 SEA FILE=CAPLUS ABB=ON PHOSPHINES/CT(L) CAT/RL
L6 148262 SEA FILE=CAPLUS ABB=ON ?ISOCYAN?/BI
L7 223 SEA FILE=CAPLUS ABB=ON URETDIONE?/BI
L8 2 SEA FILE=CAPLUS ABB=ON L5 AND L6 AND L7

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L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:427624 CAPLUS

DOCUMENT NUMBER: 140:424084

TITLE: Manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts

INVENTOR(S): Richter, Frank; Halpaap, Reinhard; Laas, Hans-Josef; Hecking, Andreas

PATENT ASSIGNEE(S): Bayer Materials science Ag, Germany

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422223	A1	20040526	EP 2003-26029	20031112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10254878	A1	20040603	DE 2002-10254878	20021125

US 2004106789	A1	20040603	US 2003-719175	20031121
BR 2003005203	A	20040831	BR 2003-5203	20031121
JP 2004175803	A2	20040624	JP 2003-393543	20031125
PRIORITY APPLN. INFO.:			DE 2002-10254878	A 20021125

OTHER SOURCE(S): MARPAT 140:424084

ED Entered STN: 27 May 2004

AB Aliphatic **polyisocyanates** comprising **uretdione** groups and having low content of byproducts (uretonimines), useful as low-viscosity internally blocked crosslinking agents for coatings, were manufactured by dimerization of aliphatic **isocyanates** in the presence of phosphines bearing ≥ 1 cycloalkyl group on the P atom. For example, in dimerization of hexamethylene **diisocyanate** at 40-100°, the **uretdione** selectivity of butyldicyclopentylphosphine catalyst at a given yield was higher than with Bu3P as catalyst.

IC ICM C07D229-00

ICS C08G018-79

CC 35-2 (Chemistry of Synthetic High Polymers)

ST aliph **isocyanate** dimerization cycloalkylphosphine catalyst;
uretdione selectivity hexamethylene **diisocyanate**
dimerization cycloalkylphosphine catalyst

IT **Phosphines**

RL: CAT (Catalyst use); USES (Uses)

(cycloalkyl derivs.; manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts)

IT Dimerization catalysts

(manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as)

IT Cyclocondensation reaction catalysts

(manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts)

IT 822-06-0, Hexamethylene **diisocyanate**

RL: RCT (Reactant); RACT (Reactant or reagent)

(dimerization; manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts)

IT 7650-88-6, Tricyclopentylphosphine 84100-17-4 691413-65-7

RL: CAT (Catalyst use); USES (Uses)

(manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts)

IT 75-13-8DP, **Isocyanic** acid, aliphatic esters, polymers

RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of **polyisocyanates** containing **uretdione** groups using cycloalkylphosphines as dimerization catalysts)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:227345 CAPLUS

DOCUMENT NUMBER: 128:295184

TITLE: Manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of catalysts and catalyst poisons

INVENTOR(S): Sugimoto, Kenji

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10095823	A2	19980414	JP 1996-253314	19960925

PRIORITY APPLN. INFO.: JP 1996-253314 19960925

OTHER SOURCE(S): MARPAT 128:295184

ED Entered STN: 22 Apr 1998

AB Title **polyisocyanates** (**isocyanurate** trimer content $\leq 10\%$; dimer content and linear trimer content of **uretdiones** $\geq 60\%$ and $\leq 30\%$, resp.), useful for curing agents, are manufactured by dimerizing aliphatic **diisocyanates** and/or alicyclic **diisocyanates** at -10° to 120° in the presence of catalysts (X2N)3P (X = C1-6 alkyl), stopping the reaction at conversion $\leq 35\%$ using catalyst poisons QC02H and/or HO2C(CH2)nCO2H (Q = C9-21 alkyl; n = 4-11), and distilling the reaction products to remove unreacted **diisocyanates**. Thus, 500 g HDI was oligomerized at 80° in the presence of 2.5 g tris(diethylamino)phosphine (I), mixed with 1.05-fold (mol, based on I) capric acid (II) when conversion reached 20%, incubated at 80° , and distilled to give an unreacted HDI not containing I and II for recycling. The obtained **polyisocyanate** showed viscosity 50 mPa-s at 25° , NCO group content 24.0%, **isocyanurate** (d.p. ≥ 3) content 4%, dimer and trimer content of **uretdione** 70% and 20%, resp.

IC ICM C08G018-02
ICS C07D229-00

CC 35-2 (Chemistry of Synthetic High Polymers)

ST trisdiethylaminophosphine catalyst **uretdione**
polyisocyanate manuf; capric acid catalyst poison HDI dimer

IT **Phosphines**
RL: CAT (Catalyst use); USES (Uses)
(amino groups-containing, catalyst; manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of phosphine catalysts and catalyst poisons)

IT Carboxylic acids, uses
RL: CAT (Catalyst use); USES (Uses)
(catalyst; manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of phosphine catalysts and catalyst poisons)

IT Fatty acids, uses
RL: CAT (Catalyst use); USES (Uses)
(manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of phosphine catalysts and catalyst poisons)

IT Polymerization catalysts
(oligomerization; manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of phosphine catalysts and catalyst poisons)

IT 57-10-3, Palmitinic acid, uses 57-11-4, Stearic acid, uses 111-20-6, Sebacic acid, uses 112-85-6, Behenic acid 124-04-9, Adipic acid, uses 143-07-7, Lauric acid, uses 334-48-5, Capric acid 505-52-2, Brassylic acid 544-63-8, Myristic acid, uses 693-23-2, Dodecanedioic acid 2283-11-6, Tris(diethylamino)phosphine
RL: CAT (Catalyst use); USES (Uses)
(manufacture of **uretdione** groups-containing **polyisocyanates** using specific combination of phosphine catalysts and catalyst poisons)

IT 28182-81-2P, Hexamethylene **diisocyanate** homopolymer
53880-05-0P, IPDI homopolymer
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(oligomeric; manufacture of **uretdione** groups-containing

polyisocyanates using specific combination of phosphine catalysts and catalyst poisons)

=> fil reg; d stat que l61; d stat que l63
FILE 'REGISTRY' ENTERED AT 13:00:01 ON 27 MAY 2005
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STRUCTURE FILE UPDATES: 26 MAY 2005 HIGHEST RN 851232-97-8
DICTIONARY FILE UPDATES: 26 MAY 2005 HIGHEST RN 851232-97-8

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

L50			STR		
O=C=N			O=C=N		
1 2 3			4 5 6		

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 2
CONNECT IS M2 RC AT 3
CONNECT IS E2 RC AT 5
CONNECT IS M2 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

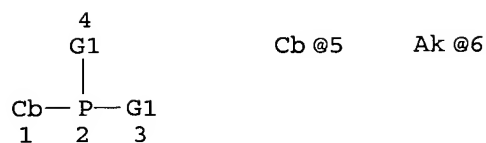
STEREO ATTRIBUTES: NONE

L61 78835 SEA FILE=REGISTRY SSS FUL L50

100.0% PROCESSED 81277 ITERATIONS
SEARCH TIME: 00.00.01

78835 ANSWERS

L52 STR



VAR G1=5/6

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 2

CONNECT IS E1 RC AT 6

DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 1 *> carbocycles at nodes 185 are saturated*

GGCAT IS SAT AT 5

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L54 1120038 SEA FILE=REGISTRY ABB=ON P/ELS AND RSD/FA

L56 15190 SEA FILE=REGISTRY ABB=ON C H P/ELF AND 3/ELC.SUB

L57 114810 SEA FILE=REGISTRY ABB=ON C H O P/ELF AND 4/ELC.SUB

L58 99690 SEA FILE=REGISTRY ABB=ON (L56 OR L57) AND L54

L63 146 SEA FILE=REGISTRY SUB=L58 SSS FUL L52

100.0% PROCESSED 99688 ITERATIONS

146 ANSWERS

SEARCH TIME: 00.00.01

=> fil capl; d que nos l66

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FILE COVERS 1907 - 27 May 2005 VOL 142 ISS 23

FILE LAST UPDATED: 26 May 2005 (20050526/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

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L50          STR
L52          STR
L54      1120038 SEA FILE=REGISTRY ABB=ON  P/ELS AND RSD/FA
L56      15190 SEA FILE=REGISTRY ABB=ON  C H P/ELF AND 3/ELC.SUB
L57      114810 SEA FILE=REGISTRY ABB=ON  C H O P/ELF AND 4/ELC.SUB
L58      99690 SEA FILE=REGISTRY ABB=ON  (L56 OR L57) AND L54
L61      78835 SEA FILE=REGISTRY SSS FUL L50
L63      146 SEA FILE=REGISTRY SUB=L58 SSS FUL L52
L64      73100 SEA FILE=CAPLUS ABB=ON  L61
L65      1751 SEA FILE=CAPLUS ABB=ON  L63
L66      13 SEA FILE=CAPLUS ABB=ON  L65 AND L64

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=> d ibib ed abs hitstr l66 1-13

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L66 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:158581 CAPLUS
DOCUMENT NUMBER: 142:263521
TITLE: Microencapsulated catalyst-ligand system,
        microencapsulation of catalyst-ligand, and reactions
        using the catalyst-ligand system
INVENTOR(S): Pears, David Alan; Treacher, Kevin Edward; Nisar,
              Mohammed
PATENT ASSIGNEE(S): Avecia Limited, UK
SOURCE: PCT Int. Appl., 48 pp.
        CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005016510	A1	20050224	WO 2004-GB3504	20040813
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: GB 2003-19071 A 20030814

ED Entered STN: 24 Feb 2005

AB A microencapsulated catalyst-ligand system is prepared by dissolving or dispersing a catalyst and/or a ligand in a first phase (organic phase), dispersing the first phase in a second, continuous phase (aqueous phase) to form an emulsion, reacting ≥ 1 microcapsule wall-forming materials at the interface between the dispersed first phase and the continuous second phase to form a microcapsule polymer shell encapsulating the dispersed first phase core and when the first phase contains only a catalyst or a ligand, treating the microcapsules with the remaining ligand or catalyst component of the catalyst-ligand system. The catalyst is preferably a transition metal catalyst and the ligand is preferably an

organic P-containing ligand. The encapsulated catalyst-ligand system may be used for conventional catalyzed reactions such as a Suzuki coupling reaction. The encapsulated catalyst-ligand system may be recovered from the reaction medium and re-cycled.

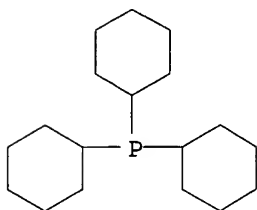
IT 2622-14-2, Tricyclohexylphosphine

RL: CAT (Catalyst use); USES (Uses)

(ligand; microencapsulated Pd acetate-P-containing ligand system for Suzuki reaction)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 57029-40-0P, Polymethylene polyphenylene isocyanate-TDI copolymer

103188-89-2P, MDI-polymethylene polyphenylene isocyanate copolymer

RL: IMF (Industrial manufacture); PREP (Preparation)

(ligand; microencapsulated Pd acetate-P-containing ligand system for Suzuki reaction)

RN 57029-40-0 CAPLUS

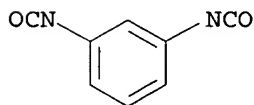
CN Isocyanic acid, polymethylenepolyphenylene ester, polymer with 1,3-diisocyanatomethylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 26471-62-5

CMF C9 H6 N2 O2

CCI IDS



D1-Me

CM 2

CRN 9016-87-9

CMF Unspecified

CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 103188-89-2 CAPLUS

CN Isocyanic acid, polymethylenepolyphenylene ester, polymer with 1,1'-methylenebis[4-isocyanatobenzene] (9CI) (CA INDEX NAME)

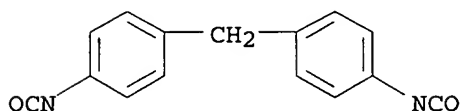
CM 1

CRN 9016-87-9
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 101-68-8
CMF C15 H10 N2 O2



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:470332 CAPLUS

DOCUMENT NUMBER: 141:24141

TITLE: Uretdione group-containing polyisocyanates with low monomer content

INVENTOR(S): Richter, Frank; Halpaap, Reinhard; Laas, Hans Josef; Hecking, Andreas

PATENT ASSIGNEE(S): Bayer Materialscience A.-G., Germany

SOURCE: Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1426393	A2	20040609	EP 2003-27009	20031122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004110915	A1	20040610	US 2003-726359	20031203
BR 2003005411	A	20040831	BR 2003-5411	20031204
JP 2004182991	A2	20040702	JP 2003-406969	20031205
PRIORITY APPLN. INFO.:			DE 2002-10256798	A 20021205

ED Entered STN: 10 Jun 2004

AB Polyisocyanates with >50 mol% uretdione content and low monomer content (<0.3%) that remained <0.5% after 6-mo storage at 50° are prepared by oligomerization of an organic isocyanate at ≤40° in the presence of a trialkylphosphine-containing catalyst to give 1-80% conversion of free NCO groups. Thus, oligomerization of HDI at 40° in the presence of butyldicyclopentylphosphine gave a polyisocyanate with viscosity 106 mPas, free HDI 0.08% and uretdione content 74 mol%. After 6-mo. storage at 50°, the free HDI content was 0.26%, indicating stability of the uretdione groups. The polyisocyanates can be used in the preparation of polyurethanes, coatings, and adhesives.

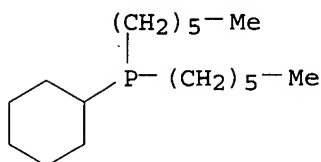
IT 84100-17-4, Cyclohexyldihexylphosphine 691413-65-7

RL: CAT (Catalyst use); USES (Uses)

(in manufacture of uretdione group-containing polyisocyanates with improved storage stability)

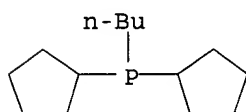
RN 84100-17-4 CAPLUS

CN Phosphine, cyclohexyldihexyl- (9CI) (CA INDEX NAME)



RN 691413-65-7 CAPLUS

CN Phosphine, butyldicyclopentyl- (9CI) (CA INDEX NAME)



IT 28182-81-2P, Hexamethylene diisocyanate homopolymer

RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)

(oligomeric, uretdione group-containing; manufacture of uretdione group-containing

polyisocyanates with improved storage stability)

RN 28182-81-2 CAPLUS

CN Hexane, 1,6-diisocyanato-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 822-06-0

CMF C8 H12 N2 O2

OCN- $(\text{CH}_2)_6$ -NCO

L66 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:427624 CAPLUS

DOCUMENT NUMBER: 140:424084

TITLE: Manufacture of polyisocyanates containing uretdione groups using cycloalkylphosphines as dimerization catalysts

INVENTOR(S): Richter, Frank; Halpaap, Reinhard; Laas, Hans-Josef; Hecking, Andreas

PATENT ASSIGNEE(S): Bayer Materialscience Ag, Germany

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

EP 1422223	A1	20040526	EP 2003-26029	20031112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10254878	A1	20040603	DE 2002-10254878	20021125
US 2004106789	A1	20040603	US 2003-719175	20031121
BR 2003005203	A	20040831	BR 2003-5203	20031121
JP 2004175803	A2	20040624	JP 2003-393543	20031125
PRIORITY APPLN. INFO.:			DE 2002-10254878	A 20021125

OTHER SOURCE(S): MARPAT 140:424084

ED Entered STN: 27 May 2004

AB Aliphatic polyisocyanates comprising uretdione groups and having low content of byproducts (uretonimines), useful as low-viscosity internally blocked crosslinking agents for coatings, were manufactured by dimerization of aliphatic isocyanates in the presence of phosphines bearing ≥ 1 cycloalkyl group on the P atom. For example, in dimerization of hexamethylene diisocyanate at 40-100°, the uretdione selectivity of butyldicyclopentylphosphine catalyst at a given yield was higher then with Bu₃P as catalyst.

IT 822-06-0, Hexamethylene diisocyanate

RL: RCT (Reactant); RACT (Reactant or reagent)

(dimerization; manufacture of polyisocyanates containing uretdione groups using cycloalkylphosphines as dimerization catalysts)

RN 822-06-0 CAPLUS

CN Hexane, 1,6-diisocyanato- (9CI) (CA INDEX NAME)

OCN-(CH₂)₆-NCO

IT 7650-88-6, Tricyclopentylphosphine 84100-17-4

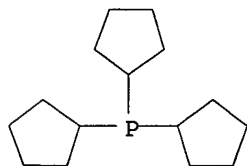
691413-65-7

RL: CAT (Catalyst use); USES (Uses)

(manufacture of polyisocyanates containing uretdione groups using cycloalkylphosphines as dimerization catalysts)

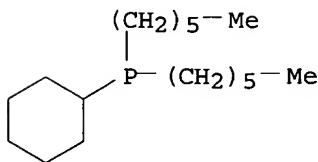
RN 7650-88-6 CAPLUS

CN Phosphine, tricyclopentyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

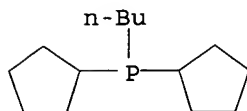


RN 84100-17-4 CAPLUS

CN Phosphine, cyclohexyldihexyl- (9CI) (CA INDEX NAME)



RN 691413-65-7 CAPLUS
CN Phosphine, butyldicyclopentyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:549324 CAPLUS

DOCUMENT NUMBER: 131:145297

TITLE: One-liquid moisture-curable urethane compositions with good curability and storability

INVENTOR(S): Araki, Kiminori; Ishikawa, Kazunori

PATENT ASSIGNEE(S): The Yokohama Rubber Co., Ltd., Japan

SOURCE: PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

checked

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9942525	A1	19990826	WO 1999-JP751	19990219
W: JP, KR, US				
US 6180713	B1	20010130	US 1999-403276	19991018
PRIORITY APPLN. INFO.:			JP 1998-37610	A 19980219
			WO 1999-JP751	W 19990219

ED Entered STN: 31 Aug 1999

AB The urethane compns. contain a urethane polymer and an amine catalyst, wherein 100 parts of the urethane polymer is blended with 0.002-50 parts of a phosphorous acid ester compound, a phosphonous acid ester compound, a phosphinous acid ester compound, a phosphine compound or a mixture thereof. These compns. have an improved storage stability and the catalytic activity thereof is not deteriorated even though amine catalysts having a dimethylamino structure and showing a high catalytic activity are employed therein. Blending polyether triol (mol. weight 5000) with polyether diol (mol. weight 2000) at 6/4 ratio, reacting with 4,4'-MDI at NCO/OH ratio 1.7 and 80° for 36 h, and mixing the resulting prepolymer 100. DOP 30, carbon black 70, bis(2-dimethylaminoethyl) ether 0.04, and Ph3P 0.002 part gave a composition with storability (as viscosity) 600 and 630 Ps and curability (20°, 65% RH) 40 and 42 min, at 20° after 24 h and 3 mo, resp.

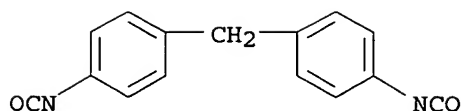
IT 101-68-8D, 4,4'-MDI, polyether polyurethanes

RL: POF (Polymer in formulation); PRP (Properties); USES (Uses)

(one-liquid moisture-curable urethane compns. with good curability and storability)

RN 101-68-8 CAPLUS

CN Benzene, 1,1'-methylenebis[4-isocyanato- (9CI) (CA INDEX NAME)



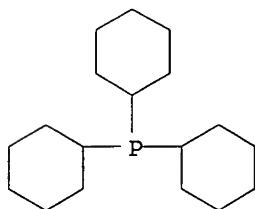
IT 2622-14-2, Tricyclohexylphosphine

RL: MOA (Modifier or additive use); USES (Uses)

(storage stabilizer; one-liquid moisture-curable urethane compns. with good curability and storability)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:206981 CAPLUS

DOCUMENT NUMBER: 130:313248

TITLE: Acrylic resin compositions for ordinary temperature-curable coatings

INVENTOR(S): Sugioka, Takuo

PATENT ASSIGNEE(S): Nippon Shokubai Kagaku Kogyo Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11080291	A2	19990326	JP 1997-240021	19970904
PRIORITY APPLN. INFO.:			JP 1997-240021	19970904

OTHER SOURCE(S): MARPAT 130:313248

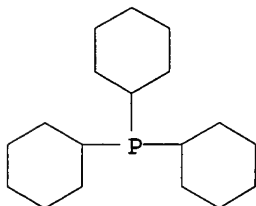
ED Entered STN: 01 Apr 1999

AB The title compns. contain resins involving (A) solid compds. (or having viscosity at 25° ≥100 P) comprising terminal or side-chain (meth)acryloyl groups, and (B) radically polymerizable compds. showing viscosity at 25° ≤10 P, at weight ratio A/B = 10/90-90/10, (C) P compds. R1R2R3P [R1-R3 = C1-10 alkyl, (C1-10 alkyl-substituted) Ph, (C1-10 alkyl-substituted) naphthyl], (D) enol-type β-diketones, and (E) redox-active organic Co compds. selected from organic acid Co salts and/or organic Co complexes. The compns. show min. discoloration and have uniform curability and give coatings with good mech. strength and resistance to corrosion, chems., and hot H2O. Thus, esterifying bisphenol-type epoxy resin (2500 g YD 901 and 580 g YD 127) with 750 g methacrylic acid gave a vinyl ester, which was mixed with 2100 g styrene and 0.02%

4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl to give a vinyl ester resin having acid value 5.0 mg-KOH/g. A composition containing the resin, Co octenoate 0.0140, K octenoate 0.0400, Ca octenoate 0.0240, and Me acetylacetate 0.2000% (based on the resin) was mixed with 1.0% (based on the composition) of a 55% MEK peroxide solution (Kayamek M) and applied onto a glass plate to give a transparent coating, which was not tacky after 2 h in the air. A cured product of the composition had min. color change after soaking in hot (100°) H₂O for 2000 h.

IT 2622-14-2, Tricyclohexyl phosphine
RL: CAT (Catalyst use); USES (Uses)
((meth)acryloyl-containing resin compns. for ordinary temperature-curable and hot water-resistant coatings)

RN 2622-14-2 CAPLUS
CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

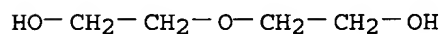


IT 223471-71-4P, Dipropylene glycol-HDI-2-Hydroxypropyl methacrylate-Styrene copolymer
RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
((meth)acryloyl-containing resin compns. for ordinary temperature-curable and hot water-resistant coatings)

RN 223471-71-4 CAPLUS
CN 2-Propenoic acid, 2-methyl-, 2-hydroxypropyl ester, polymer with 1,6-diisocyanatohexane, ethenylbenzene and oxybis[propanol] (9CI) (CA INDEX NAME)

CM 1

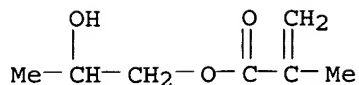
CRN 25265-71-8
CMF C6 H14 O3
CCI IDS



2 (D1-Me)

CM 2

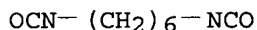
CRN 923-26-2
CMF C7 H12 O3



CM 3

CRN 822-06-0

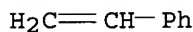
CMF C8 H12 N2 O2



CM 4

CRN 100-42-5

CMF C8 H8



L66 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:333008 CAPLUS

DOCUMENT NUMBER: 125:127644

TITLE: Method for obtaining improved image contrast in migration imaging members

INVENTOR(S): Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths, Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron, Marie-Eve

PATENT ASSIGNEE(S): Xerox Corp., USA

SOURCE: U.S., 147 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5514505	A	19960507	US 1995-441360	19950515
CA 2169980	AA	19961116	CA 1996-2169980	19960221
CA 2169980	C	20010424		
JP 08314240	A2	19961129	JP 1996-113456	19960508
EP 743573	A2	19961120	EP 1996-303359	19960514
EP 743573	A3	19970305		
EP 743573	B1	20000906		

R: DE, FR, GB

PRIORITY APPLN. INFO.: US 1995-441360 A 19950515

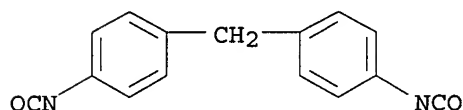
OTHER SOURCE(S): MARPAT 125:127644

ED Entered STN: 08 Jun 1996

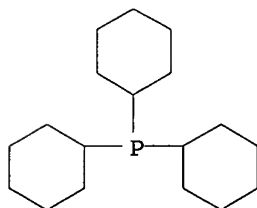
AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material

present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.

IT 101-68-8 2622-14-2, Tricyclohexylphosphine
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(transparentizing agent for electrophotog. migration imaging members)
RN 101-68-8 CAPLUS
CN Benzene, 1,1'-methylenebis[4-isocyanato- (9CI) (CA INDEX NAME)



RN 2622-14-2 CAPLUS
CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L66 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:569981 CAPLUS
DOCUMENT NUMBER: 109:169981
TITLE: Carbon-carbon coupling of styrene with
 α,ω -diisocyanates, induced and catalyzed
by nickel(0)
AUTHOR(S): Hoberg, Heinz; Hernandez, Elisa; Guhl, Dieter
CORPORATE SOURCE: Max-Planck Inst. Kohlenforsch., Muelheim, D-4330, Fed.
Rep. Ger.
SOURCE: Journal of Organometallic Chemistry (1988), 339(1-2),
213-21
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 109:169981
ED Entered STN: 12 Nov 1988
AB The reaction of $\text{OCN}(\text{CH}_2)_6\text{NCO}$ with styrene at the Ni0-
tricyclohexylphosphine system is dependent on the molar ratio to give
either the mono- or the bisazanickele derivative Under certain conditions the

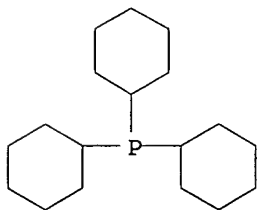
normally stoichiometric reaction changes into one which is catalytic. In a regioselective C-C coupling reaction N,N'-(hexanediyl)biscinnamamide is formed after about 7 catalytic cycles. Spectroscopic and chemical methods were used to identify the structures. Some special features of the C-C coupling reactions and the mechanism of the catalysis are described.

IT 2622-14-2, Tricyclohexylphosphine

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dicyclooctadienyl nickel, hexamethylene diisocyanate, in styrene)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 822-06-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dicyclooctadienyl nickel, tricyclohexylphosphine and styrene)

RN 822-06-0 CAPLUS

CN Hexane, 1,6-diisocyanato- (9CI) (CA INDEX NAME)

OCN-(CH₂)₆-NCO

L66 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:122562 CAPLUS

DOCUMENT NUMBER: 84:122562

TITLE: Chloral copolymers

INVENTOR(S): Vogl, Otto F.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: U.S., 24 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3932318	A	19760113	US 1974-530438	19741206
GB 1151002	A	19690507	GB 1967-1151002	19670619
US 3668184	A	19720606	US 1969-886739	19691219
US 3775371	A	19731127	US 1972-227684	19720218
US 3917546	A	19751104	US 1973-352387	19730418
PRIORITY APPLN. INFO.:			US 1966-558631	A2 19660620
			US 1966-580217	A2 19660919
			US 1968-731622	A2 19680523
			US 1969-886739	A3 19691219
			US 1972-227684	A3 19720218

US 1973-352387

A3 19730418

ED Entered STN: 12 May 1984

AB Addition copolymers of chloral (I) with organic isocyanates and/or ketenes are prepared via cryotachensic polymerization, i.e., polymerization by cooling below the

threshold polymerization temperature during which the homogeneous polymerization mixture remains

quiescent to form a continuous gel which ultimately converts to a high polymer, in the presence of initiators, such as tert-BuOLi [1907-33-1], phosphines, and phosphoniums. The polymerization may be conducted in a mold. Thus, a mixture of 30 g I and 2.7 g phenyl isocyanate (II) was heated to 65° and 0.4 ml 1M tert-BuOLi in cyclohexane added to give a homogeneous mixture having threshold polymerization temperature 47°. The

mixture

was allowed to become quiescent and polymerized by cooling at -50° for 1 hr to give a I-II copolymer [25838-94-2] film which was insol. in organic solvents and had tensile strength 6720 psi, elongation at break 8.8%, and 5% weight loss temperature (on heating at 6°/min in N) 197-200°.

Glass-fiber reinforced I-copolymers were obtained similarly and were noncombustible with good mech. properties. Phosphine and phosphonium initiators were also prepared and used to give clear transparent sheets of I-p-chlorophenyl isocyanate copolymer [25838-94-2].

IT 26899-05-8 57950-94-4 57950-95-5

57951-10-7 57951-13-0 58067-49-5

RL: USES (Uses)

(cryotachensic manufacture and properties of)

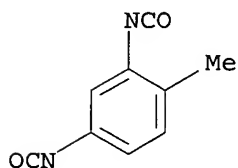
RN 26899-05-8 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 2,4-diisocyanato-1-methylbenzene, 1-isocyanatobutane and isocyanatobenzene (9CI) (CA INDEX NAME)

CM 1

CRN 584-84-9

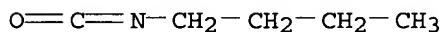
CMF C9 H6 N2 O2



CM 2

CRN 111-36-4

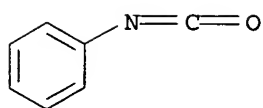
CMF C5 H9 N O



CM 3

CRN 103-71-9

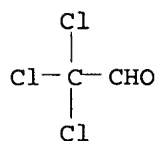
CMF C7 H5 N O



CM 4

CRN 75-87-6

CMF C2 H Cl3 O



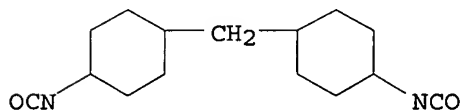
RN 57950-94-4 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,1'-methylenebis[4-isocyanatocyclohexane] (9CI) (CA INDEX NAME)

CM 1

CRN 5124-30-1

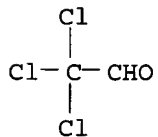
CMF C15 H22 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



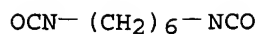
RN 57950-95-5 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,6-diisocyanatohexane (9CI) (CA INDEX NAME)

CM 1

CRN 822-06-0

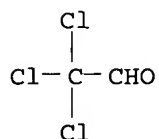
CMF C8 H12 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



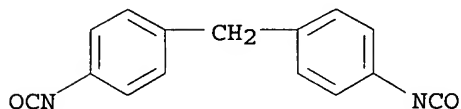
RN 57951-10-7 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,1'-methylenebis[4-isocyanatobenzene] (9CI) (CA INDEX NAME)

CM 1

CRN 101-68-8

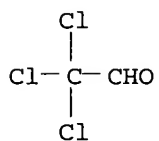
CMF C15 H10 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



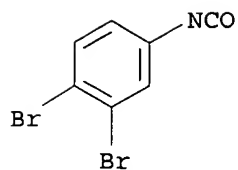
RN 57951-13-0 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,2-dibromo-4-isocyanatobenzene, 1,6-diisocyanatohexane and diphenylethenone (9CI) (CA INDEX NAME)

CM 1

CRN 36647-47-9

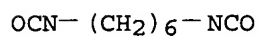
CMF C7 H3 Br2 N O



CM 2

CRN 822-06-0

CMF C8 H12 N2 O2



CM 3

CRN 525-06-4

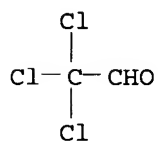
CMF C14 H10 O



CM 4

CRN 75-87-6

CMF C2 H Cl3 O



RN 58067-49-5 CAPLUS

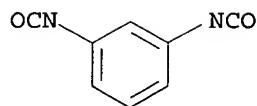
CN Acetaldehyde, trichloro-, polymer with 1,3-diisocyanatomethylbenzene (9CI)
(CA INDEX NAME)

CM 1

CRN 26471-62-5

CMF C9 H6 N2 O2

CCI IDS

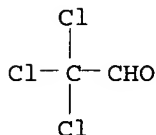


D1- Me

CM 2

CRN 75-87-6

CMF C2 H Cl3 O

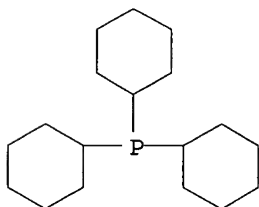


IT 2622-14-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L66 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:45227 CAPLUS

DOCUMENT NUMBER: 84:45227

TITLE: Chloral copolymers

INVENTOR(S): Vogl, Otto F.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: U.S., 23 pp. Division of U.S. 3,775,371.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3917546	A	19751104	US 1973-352387	19730418
US 3668184	A	19720606	US 1969-886739	19691219

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X

Nyalley

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Page 105

US 3775371	A	19731127	US 1972-227684	19720218
US 3932318	A	19760113	US 1974-530438	19741206
PRIORITY APPLN. INFO.:			US 1969-886739	A3 19691219
			US 1972-227684	A3 19720218
			US 1966-558631	A3 19660620
			US 1966-580217	A2 19660919
			US 1968-731622	A2 19680523
			US 1973-352387	A3 19730418

ED Entered STN: 12 May 1984

AB Chloral (I) [75-87-6] was copolymd. with ≥ 1 isocyanate, isothiocyanate, diisocyanate, diisothiocyanate, or ketene compound to form nonflammable copolymers. The monomer mixture was prepared at a temperature above

the threshold polymerization temperature of the mixture, cooled below the threshold

polymerization temperature, and kept quiescent during the polymerization

Thus, a mixture of 30

g I and 2.7 g Ph isocyanate was heated to 65°, and the quiescent mixture was polymerized 1 hr at -50° in the presence of 0.4 ml 1M Li tert-butoxide in cyclohexane to yield the insol. chloral-phenyl isocyanate copolymer [25838-94-2].

IT 26899-05-8P 57950-94-4P 57950-95-5P

57951-10-7P 57951-13-0P 58067-49-5P

RL: PREP (Preparation)

(preparation of)

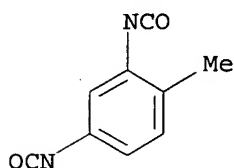
RN 26899-05-8 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 2,4-diisocyanato-1-methylbenzene, 1-isocyanatobutane and isocyanatobenzene (9CI) (CA INDEX NAME)

CM 1

CRN 584-84-9

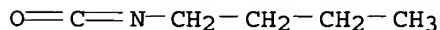
CMF C9 H6 N2 O2



CM 2

CRN 111-36-4

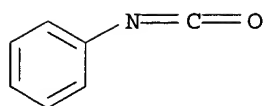
CMF C5 H9 N O



CM 3

CRN 103-71-9

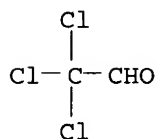
CMF C7 H5 N O



CM 4

CRN 75-87-6

CMF C2 H Cl3 O



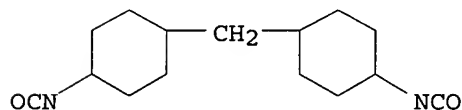
RN 57950-94-4 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,1'-methylenebis[4-isocyanatocyclohexane] (9CI) (CA INDEX NAME)

CM 1

CRN 5124-30-1

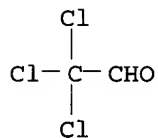
CMF C15 H22 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



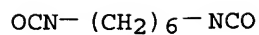
RN 57950-95-5 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,6-diisocyanatohexane (9CI) (CA INDEX NAME)

CM 1

CRN 822-06-0

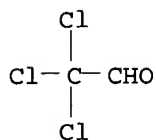
CMF C8 H12 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



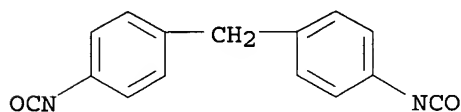
RN 57951-10-7 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,1'-methylenebis[4-isocyanatobenzene] (9CI) (CA INDEX NAME)

CM 1

CRN 101-68-8

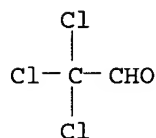
CMF C15 H10 N2 O2



CM 2

CRN 75-87-6

CMF C2 H Cl3 O



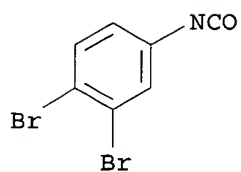
RN 57951-13-0 CAPLUS

CN Acetaldehyde, trichloro-, polymer with 1,2-dibromo-4-isocyanatobenzene, 1,6-diisocyanatohexane and diphenylethenone (9CI) (CA INDEX NAME)

CM 1

CRN 36647-47-9

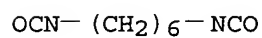
CMF C7 H3 Br2 N O



CM 2

CRN 822-06-0

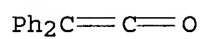
CMF C8 H12 N2 O2



CM 3

CRN 525-06-4

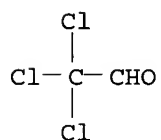
CMF C14 H10 O



CM 4

CRN 75-87-6

CMF C2 H Cl3 O



RN 58067-49-5 CAPLUS

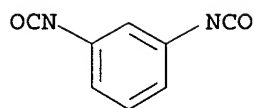
CN Acetaldehyde, trichloro-, polymer with 1,3-diisocyanatomethylbenzene (9CI)
(CA INDEX NAME)

CM 1

CRN 26471-62-5

CMF C9 H6 N2 O2

CCI IDS

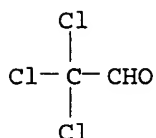


D1-Me

CM 2

CRN 75-87-6

CMF C2 H Cl3 O

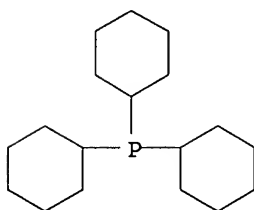


IT 2622-14-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L66 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:526926 CAPLUS

DOCUMENT NUMBER: 79:126926

TITLE: 2,4,6-Trioxo-1,3,5-oxadiazines

INVENTOR(S): Liebsch, Dietrich; Meisert, Ernst; Stopp, Gerhard

PATENT ASSIGNEE(S): Bayer A.-G.

SOURCE: U.S., 8 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

have
X

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3748329	A	19730724	US 1970-53277	19700708
PRIORITY APPLN. INFO.:			US 1967-612358	A2 19670130

ED Entered STN: 12 May 1984

AB Reaction of an organic polyisocyanate with carbon dioxide [124-38-9] in the presence of arsine or phosphine catalysts gave a 2,4,6-trioxo-1,3,5-oxadiazine derivative I, from which porous and nonporous polymers were prepared. Thus, heating 1,6-hexamethylene diisocyanate [822-06-0] 336, solid CO₂ 30 and tributylphosphine [998-40-3] 1.7g at 60.deg. for 70 min under CO₂ gave 92g yellowish oil of low viscosity. Addition of 21 parts dioxyethylamine to 78 parts this product at .leq.50.deg. and heating to 120-150.deg. until crosslinking occurred, yielded a hard, viscous foam.

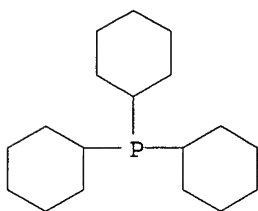
IT 2622-14-2

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for reaction of carbon dioxide with diisocyanates)

RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 50639-37-7P 50639-38-8P 50659-02-4P

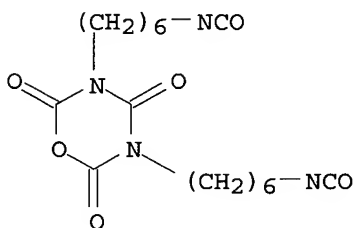
50939-86-1P

RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of, catalysts for)

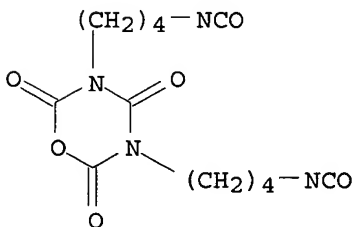
RN 50639-37-7 CAPLUS

CN 2H-1,3,5-Oxadiazine-2,4,6(3H,5H)-trione, 3,5-bis(6-isocyanatohexyl)- (9CI)
(CA INDEX NAME)



RN 50639-38-8 CAPLUS

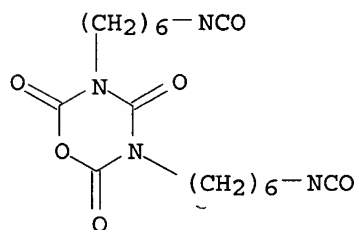
CN 2H-1,3,5-Oxadiazine-2,4,6(3H,5H)-trione, 3,5-bis(4-isocyanatobutyl)- (9CI)
(CA INDEX NAME)



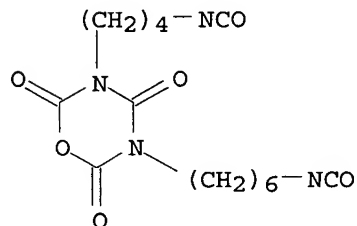
RN 50659-02-4 CAPLUS
CN 2H-1,3,5-Oxadiazine-2,4,6(3H,5H)-trione, 3,5-bis(6-isocyanatohexyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

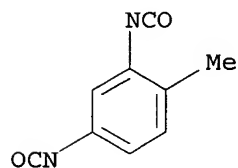
CRN 50639-37-7
CMF C17 H24 N4 O6



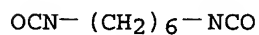
RN 50939-86-1 CAPLUS
CN 2H-1,3,5-Oxadiazine-2,4,6(3H,5H)-trione, 3-(4-isocyanatobutyl)-5-(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



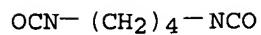
IT **584-84-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(isocyanatohexyl)trioxooxadiazine)
RN 584-84-9 CAPLUS
CN Benzene, 2,4-diisocyanato-1-methyl- (9CI) (CA INDEX NAME)



IT **822-06-0 4538-37-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbon dioxide)
RN 822-06-0 CAPLUS
CN Hexane, 1,6-diisocyanato- (9CI) (CA INDEX NAME)



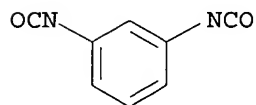
RN 4538-37-8 CAPLUS
 CN Butane, 1,4-diisocyanato- (9CI) (CA INDEX NAME)



IT 9046-11-1
 RL: USES (Uses)
 (stabilizers for, bis(isocyanatohexyl)trioxooxadiazine as)
 RN 9046-11-1 CAPLUS
 CN Hexanedioic acid, polymer with 1,3-diisocyanatomethylbenzene,
 1,2-ethanediol and 2,2'-oxybis[ethanol] (9CI) (CA INDEX NAME)

CM 1

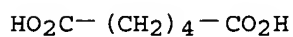
CRN 26471-62-5
 CMF C9 H6 N2 O2
 CCI IDS



D1-Me

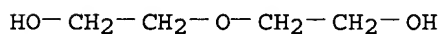
CM 2

CRN 124-04-9
 CMF C6 H10 O4



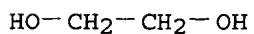
CM 3

CRN 111-46-6
 CMF C4 H10 O3



CM 4

CRN 107-21-1
 CMF C2 H6 O2



L66 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:430543 CAPLUS

DOCUMENT NUMBER: 71:30543

TITLE: Pseudohalo-metal compounds. XXVII. Formation of isocyanato complexes from complex metal azides and carbon monoxide

AUTHOR(S): Beck, Wolfgang; Fehlhammer, Wolf P.; Poellmann, Peter; Schaechl, Hans

CORPORATE SOURCE: Techn. Hochsch. Muenchen, Munich, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1969), 102(6), 1976-87

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

ED Entered STN: 12 May 1984

AB L2Pd(N3)2 (where L = PPh3, tricyclohexylphosphine, Bu3P, (PhO)3P, or piperidine), (Ph3P)2MN3 [where M = Cu(I) or Ag(I)], Ph3PAuN3, (Ph3P)3MN3 [where M = Au(I), or Rh(I)] (Ph3P)4Rh2(N3)2, and (Ph3P)2Ir(CO)N3 were prepared Their properties and ir spectra are reported. The Pd, Au, Rh, and Ir complexes reacted with CO in CHCl3 or C6H6 to form the corresponding isocyanato complexes. [Ph3PPd(N3)2]2 reacted similarly to form [Ph3PPd(NCO)2]2 for which an isocyanate bridged structure is suggested. The rate of the reaction with CO was dependent on the CO partial pressure.

IT 2622-14-2DP, Phosphine, tricyclohexyl-, palladium complexes

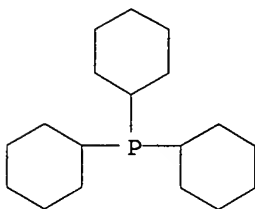
14782-11-7P 14782-12-8P 23028-35-5P

23028-39-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

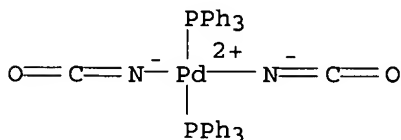
RN 2622-14-2 CAPLUS

CN Phosphine, tricyclohexyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



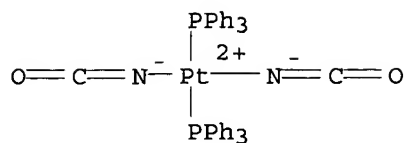
RN 14782-11-7 CAPLUS

CN Palladium, bis(cyanato-N)bis(triphenylphosphine)- (9CI) (CA INDEX NAME)



RN 14782-12-8 CAPLUS

CN Platinum, bis(cyanato-N)bis(triphenylphosphine)- (9CI) (CA INDEX NAME)



RN 23028-35-5 CAPLUS

CN Arsonium, tetraphenyl-, bis(isocyanato)aurate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 44606-69-1

CMF C2 Au N2 O2

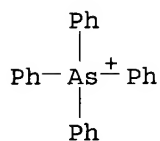
CCI CCS



CM 2

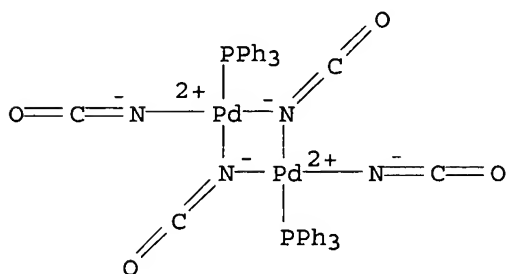
CRN 15912-80-8

CMF C24 H20 As



RN 23028-39-9 CAPLUS

CN Palladium, bis(μ-isocyanato)bis(isocyanato)bis(triphenylphosphine)di-, trans- (8CI) (CA INDEX NAME)



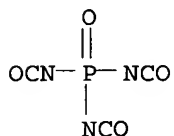
L66 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1968:25326 CAPLUS

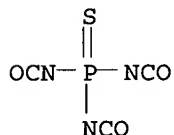
DOCUMENT NUMBER: 68:25326

TITLE: Nuclear magnetic resonance of phosphorus compounds.
 XVI. Reactions of phosphorus(III) compounds with
 sulfur dioxide

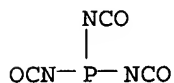
AUTHOR(S): Fluck, Ekkehard; Binder, Herbert
CORPORATE SOURCE: Univ. Heidelberg, Heidelberg, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie
(1967), 354(3-4), 139-48
CODEN: ZAACAB; ISSN: 0044-2313
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 12 May 1984
AB Trivalent P compds., including P halides, organophosphines, phosphites, aminophosphines, and PH₃ (28 compds.) were oxidized by SO₂ at 50°. The reaction was followed by the ³¹P-resonance spectra. The chemical shifts and coupling constants of the oxidation products are reported.
IT 1858-24-8 17382-94-4
RL: PRP (Properties)
(nuclear magnetic resonance of phosphorus-31 in)
RN 1858-24-8 CAPLUS
CN Phosphoric triisocyanate (9CI) (CA INDEX NAME)



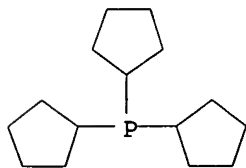
RN 17382-94-4 CAPLUS
CN Phosphorothioic triisocyanate (9CI) (CA INDEX NAME)



IT 1782-09-8 7650-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by sulfur dioxide, mechanism of)
RN 1782-09-8 CAPLUS
CN Phosphorous triisocyanate (9CI) (CA INDEX NAME)



RN 7650-88-6 CAPLUS
CN Phosphine, tricyclopentyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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L66 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:478610 CAPLUS

DOCUMENT NUMBER: 67:78610

TITLE: Reaction of trans-[Ni(PR₃)₂X₂] complexes with phosphines and amines. Formation of stable five-coordinate intermediates

AUTHOR(S): Rigo, Pierluigi; Pecile, Cesare; Turco, Aldo

CORPORATE SOURCE: Univ. Padua, Padua, Italy

SOURCE: Inorganic Chemistry (1967), 6(9), 1636-40

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 12 May 1984

AB Tertiary phosphines, PR₃, do not yield 5-coordinated adducts by reaction with the planar complexes trans-Ni(PR₃)₂X₂ (PR₃ = PEt₃, PEt₂Ph and X = Cl, Br, NCO, NCS; PR₃ = PEtCy, PEtCy₂, PCy₃ (Cy = cyclohexyl) and X = Cl, Br, NCS; PR₃ = PEtPh₂ and X = NCS). However, PEt₃ and PEt₂Ph immediately replace PCy₃ and PEtCy₂ in the reactions with the halide complexes. Since the reverse reactions are also observable, the result of these reactions is actually the exchange of the coordinated by the free phosphine. However, the reactions of the complexes trans-Ni(PR₃)₂(CN)₂ with the corresponding phosphines give in solution, the stable 5-coordinated intermediates as shown by the visible spectra. The compound Ni(PEt₂Ph)₃(CN)₂ has also been isolated in the solid state. The 5-coordinate compds. are discussed in terms of the binding properties of the ligands, the kinetic behavior toward the substitution, and their thermodynamic stability. With EtNH₂ and BuNH₂ only substitution reactions occur.

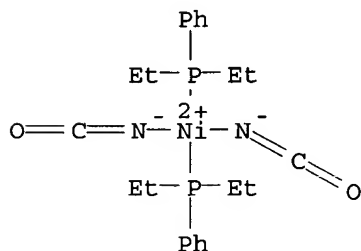
IT 16581-05-8 19262-01-2D, Phosphine, cyclohexyldiethyl-, nickel complexes 46392-44-3D, Phosphine, dicyclohexylethyl-, nickel complexes

RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reactions of, with amines and phosphines)

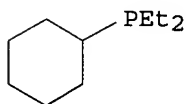
RN 16581-05-8 CAPLUS

CN Nickel, bis(diethylphenylphosphine)bis(isocyanato)-, trans- (8CI) (CA INDEX NAME)



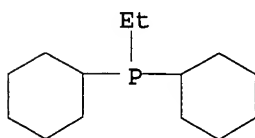
RN 19262-01-2 CAPLUS

CN Phosphine, cyclohexyldiethyl- (8CI, 9CI) (CA INDEX NAME)



RN 46392-44-3 CAPLUS

CN Phosphine, dicyclohexylethyl- (6CI, 9CI) (CA INDEX NAME)



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